Introduction to Programming with Fortran

Ian D. Chivers and Jane Sleightholme

Introduction to Programming with Fortran

With Coverage of Fortran 90, 95, 2003, and 77

Springer

Ian D. Chivers, BSc, PGCEd, MSc, MBCS
Rhymney Consulting
UK

Jane Sleightholme, MSc, MBCS
Kings College London
UK

British Library Cataloguing in Publication Data
A catalogue record for this book is available from the British Library

Library of Congress Control Number: 2005931518

ISBN-10: 1-84628-053-2 eISBN 1-84628-054-0 Printed on acid-free paper
ISBN-13: 978-1-84628-053-5

© Springer-Verlag London Limited 2006

Apart from any fair dealing for the purposes of research or private study, or criticism or review, as permitted under the Copyright, Designs and Patents Act 1988, this publication may only be reproduced, stored or transmitted, in any form or by any means, with the prior permission in writing of the publishers, or in the case of reprographic reproduction in accordance with the terms of licences issued by the Copyright Licensing Agency. Enquiries concerning reproduction outside those terms should be sent to the publishers.

The use of registered names, trademarks, etc. in this publication does not imply, even in the absence of a specific statement, that such names are exempt from the relevant laws and regulations and therefore free for general use.

The publisher makes no representation, express or implied, with regard to the accuracy of the information contained in this book and cannot accept any legal responsibility or liability for any errors or omissions that may be made.

Printed in the United States of America (MVY)

9 8 7 6 5 4 3 2 1

Springer Science+Business Media
springeronline.com

Acknowlegement

The material in the book has evolved firstly from our combined experience of working in Computing Services within the University of London at

- King's College, IDC (1986–2002) and JS (1985 to date)
- Chelsea College, JS (1978–1985)
- Imperial College, IDC (1978–1986)

in the teaching, advice and support of Fortran and related areas, and secondly in the provision of commercial training courses. The following are some of the organisations we've provided training for:

- AWE, Aldermaston.
- Centre for Ecology and Hydrology, Wallingford.
- Environment Agency, Worthing.
- The Met Office, Bracknell and Exeter.
- QinetiQ, Farnborough.
- Rolls Royce, Derby.
- Veritas DGC Ltd., Crawley.
- Westland Helicopters, Yeovil.

The examples in the book are based on what will work with compilers that support the Fortran 90 and 95 standards and also support ISO TR 15580 and 15581. At the time of writing this book there are no compilers that fully support the Fortran 2003 standard.

Thanks are due to:

- The staff and students at King's College, Chelsea College and Imperial College.

- The people who have attended the commercial courses. Its been great fun teaching you and things have been very lively at times.
- The people on the Fortran 90 list and comp.lang.fortran. Access to the expertise of several hundred people involved in the use and development of Fortran on a daily basis across a wide range of disciplines is inestimable.
- The people at NAG for the provision of the Fortran 95 compilers and Nag Tools on the enclosed cd.
- The staff and facilities at PTR Associates. It is a pleasure training there.
- The patience of our families during the time required to develop the courses upon which this book is based and whilst preparing the camera-ready copy.
- Finally Rebecca Mowat, Joanne Cooling, Helen Desmond and Beverley Ford at Springer for their enthusiasm and encouragement!

Our King's home page is:

- http://www.kcl.ac.uk/fortran

All of the program examples can be found there.

If you would like to contact us our email addresses are:

Ian D Chivers: ian.chivers@chiversandbryan.co.uk

Jane Sleightholme: jane.sleightholme@kcl.ac.uk

Contents

1 Overview 1

2 Introduction to Computer Systems 9

2.1 The core of a computer system 10

2.1.1 Central processor unit — CPU 10

2.1.2 Memory 10

2.1.3 Bus 10

2.2 Other components of a computer system 11

2.2.1 Disks 11

2.2.2 Others 11

2.3 Software 12

2.4 Problems 13

2.5 Bibliography 13

3 Introduction to Operating Systems 15

3.1 History of operating systems 16

3.1.1 The 1940s 16

3.1.2 The 1950s 16

3.1.3 The 1960s 16

3.1.4 The 1960s and 1970s 16

3.1.5 The 1970s, 1980s, and 1990s 17

3.2 Networking 17

3.3 Problems 18

3.4 Bibliography 18

4 Introduction to Using a Computer System 19

4.1 Files 20

4.2 Editors 20

4.3 Single-user systems 20

4.4 Networked systems 20

4.5 Multiuser systems 21

4.6 Other useful things to know 21

4.7 Common methods of using computer systems to develop Fortran programs . . . 22
4.8 Bibliography . . . 23
5 Introduction to Problem Solving . . . 25
5.1 Natural language . . . 26
5.2 Artificial language . . . 27
5.2.1 Notations . . . 27
5.3 Resumé . . . 27
5.4 Algorithms . . . 28
5.4.1 Top-down . . . 28
5.4.2 Bottom-up . . . 28
5.4.3 Stepwise refinement . . . 29
5.4.4 Modular programming . . . 29
5.4.5 Object oriented programming . . . 29
5.5 Systems analysis and design . . . 30
5.5.1 Problem definition . . . 30
5.5.2 Feasibility study and fact finding . . . 30
5.5.3 Analysis . . . 31
5.5.4 Design . . . 31
5.5.5 Detailed design . . . 31
5.5.6 Implementation . . . 31
5.5.7 Evaluation and testing . . . 31
5.5.8 Maintenance . . . 32
5.6 Conclusions . . . 32
5.7 Problems . . . 32
5.8 Bibliography . . . 33
6 Introduction to Programming Languages . . . 35
6.1 Some early theoretical work . . . 36
6.2 What is a programming language? . . . 36
6.3 Program language development and engineering . . . 36
6.4 The early days . . . 36
6.4.1 Fortran — The Early Days . . . 37
6.4.2 Fortran 77 . . . 37
6.4.3 Cobol . . . 37
6.4.4 Algol . . . 38
6.5 Chomsky and program language development . . . 39
6.6 Lisp . . . 39
6.7 Snobol . . . 40
6.8 Second-generation languages . . . 40
6.8.1 PL/1 and Algol 68 . . . 40
6.8.2 Simula . . . 40
6.8.3 Pascal . . . 41

6.8.4 APL . . . 41
6.8.5 Basic . . . 41
6.8.6 C . . . 41
6.9 Some other strands in language development . . . 42
6.9.1 Abstraction, stepwise refinement and modules . . . 42
6.9.2 Structured programming . . . 42
6.9.3 Standardisation . . . 42
6.10 Ada . . . 43
6.11 Modula . . . 43
6.12 Modula 2 . . . 44
6.13 Other language developments . . . 44
6.13.1 Logo . . . 44
6.13.2 Postscript, TeX and LaTeX . . . 45
6.13.3 Prolog . . . 45
6.13.4 SQL . . . 45
6.13.5 ICON . . . 46
6.14 Object orientated programming — OOP . . . 46
6.14.1 Oberon and Oberon 2 . . . 46
6.14.2 Smalltalk . . . 47
6.14.3 C++ . . . 48
6.14.4 Java . . . 48
6.14.5 Visual Basic . . . 49
6.14.6 C# . . . 49
6.15 Fortran 90 . . . 50
6.16 Fortran 1995 . . . 51
6.17 ISO technical reports TR15580 and TR15581 . . . 52
6.18 Fortran 2003 . . . 52
6.19 DTR 19767 enhanced module facilities . . . 53
6.20 Internet resources . . . 54
6.20.1 Standards information . . . 54
6.20.2 Fortran discussion lists . . . 55
6.20.3 Other sources . . . 55
6.21 Summary . . . 56
6.22 Bibliography . . . 56
7 Introduction to Programming . . . 63
7.1 Language strengths and weaknesses . . . 64
7.2 Elements of a programming language . . . 64
7.2.1 Data description statements . . . 65
7.2.2 Control structures . . . 65
7.2.3 Data-processing statements . . . 65
7.2.4 Input and output (I/O) statements . . . 65
7.3 Variables — name, type and value . . . 68

7.4 Notes. . . . 70
7.5 Some more Fortran rules . . . 71
7.6 Fortran character set . . . 72
7.7 Good programming guidelines . . . 73
7.8 Compilers . . . 73
7.9 Program development . . . 74
7.10 Problems . . . 75
8 Arithmetic . . . 77
8.1 Rounding and truncation . . . 81
8.2 Time taken for light to travel from the Sun to Earth. . . . 83
8.3 The PARAMETER statement . . . 84
8.4 Range, precision and size of numbers . . . 85
8.5 Health warning: optional reading, beginners are advised to leave until later . . . 88
8.5.1 Selecting different INTEGER kind types . . . 90
8.5.2 Selecting different REAL kind types . . . 91
8.5.3 Specifying kind types for literal integer and real constants. . . . 91
8.5.4 Positional number systems. . . . 92
8.5.5 Bit data type and representation model . . . 92
8.5.6 Integer data type and representation model . . . 93
8.5.7 Real data type and representation model . . . 93
8.5.8 IEEE 754. . . . 94
8.5.9 Testing the numerical representation of different kind types on a system . . . 94
8.5.10 Binary representation of different integer kind type numbers . . . 98
8.5.11 Binary representation of a real number . . . 100
8.5.12 Summary of how to select the appropriate kind type . . . 101
8.6 Variable status. . . . 101
8.7 Summary . . . 101
8.8 Problems . . . 102
8.9 Bibliography . . . 105
9 Arrays 1: Some Fundamentals . . . 107
9.1 Tables of data . . . 108
9.1.1 Telephone directory . . . 108
9.1.2 Book catalogue . . . 108
9.1.3 Examination marks or results . . . 109
9.1.4 Monthly rainfall . . . 109
9.2 Arrays in Fortran . . . 110
9.3 The DIMENSION attribute. . . . 110
9.4 An index . . . 111
9.5 Control structure. . . . 111
9.6 Monthly rainfall . . . 111

9.6.1 Example 1: Rainfall . . . 112
9.7 People's weights . . . 113
9.7.1 Example 2: Setting array size with a parameter . . . 114
9.8 Summary . . . 115
9.9 Problems . . . 116

10 Arrays 2: Further Examples . . . 119
10.1 Varying the array size at run time . . . 120
10.2 Higher-dimension arrays . . . 121
10.2.1 A map . . . 121
10.2.2 Example 3: Sensible tabular output . . . 123
10.2.3 Example 4: Average of three sets of values . . . 124
10.2.4 Example 5: Booking arrangements in a theatre or cinema . . . 125
10.3 Additional forms of the DIMENSION attribute and DO loop statement . . . 126
10.3.1 Example 6: Voltage from −20 to +20 volts . . . 126
10.3.2 Example 7: Longitude from −180 to +180. . . . 127
10.3.3 Notes . . . 127
10.4 The DO loop and straight repetition. . . . 127
10.4.1 Example 8: Table of temperatures . . . 127
10.4.2 Example 9: Means and standard deviations . . . 128
10.5 Summary . . . 129
10.6 Problems . . . 130

11 Whole Array and Additional Array Features. . . . 133
11.1 Terminology. . . . 134
11.1.1 Rank . . . 134
11.1.2 Bounds . . . 134
11.1.3 Extent. . . . 134
11.1.4 Size. . . . 134
11.1.5 Shape . . . 134
11.1.6 Conformable . . . 134
11.1.7 Array element ordering. . . . 134
11.2 Whole array manipulation . . . 135
11.2.1 Assignment . . . 135
11.2.2 Expressions . . . 135
11.3 Array sections . . . 138
11.3.1 Rank 1 array example . . . 138
11.3.2 Rank 2 array example . . . 138
11.4 Array constructors . . . 140
11.4.1 Rank 1 array example — explicit values . . . 140
11.4.1.1 Rank 1 array example and implied DO loop. . . . 141
11.4.1.2 Rank 1 array example and the DOT_PRODUCT intrinsic . . . 141
11.4.2 Rank 1 example with step size of 2 in implied DO loop . . . 143

11.4.3 Rank 1 array and the SUM intrinsic function 144
11.4.4 Rank 2 arrays and the SUM intrinsic function 145
11.5 Masked array assignment and the WHERE statement 146
11.5.1 Notes 147
11.6 The FORALL statement and FORALL construct 147
11.6.1 Syntax 147
11.6.2 Array element ordering and physical and virtual memory 148
11.7 Summary 148
11.8 Problems 149
11.9 Bibliography 149

12 Output of Results 151
12.1 Integers — I format or edit descriptor 152
12.2 Reals — F format or edit descriptor 155
12.2.1 Metric and imperial conversion 156
12.2.2 Overflow and underflow 156
12.3 Reals — E format or edit descriptor 158
12.3.1 Simple E format example 159
12.4 Spaces 160
12.5 Characters — A format or edit descriptor 160
12.5.1 Headings 161
12.6 Mixed type output in a FORMAT statement 162
12.7 Common mistakes 162
12.8 OPEN (and CLOSE) 163
12.8.1 The OPEN statement 163
12.8.2 Writing 164
12.9 Repetition 165
12.10 Some more examples 167
12.11 Implied DO loops and array sections for array output 168
12.12 Formatting for a line printer 170
12.12.1 Mechanics of carriage control 171
12.12.2 Generating a new line on both line printers and terminals 172
12.13 Timing of writing formatted files 173
12.14 Timing of writing unformatted files 174
12.15 Summary 176
12.16 Problems 176

13 Reading in Data 179
13.1 Reading from the terminal or keyboard versus reading from files 180
13.2 Fixed fields on input 180
13.2.1 Integers and the I format 180
13.2.2 Reals and the F format 181
13.2.3 Reals and the E Format 182

13.3 Blanks, nulls and zeros . . . 185
13.4 Characters . . . 186
13.5 Skipping spaces and lines . . . 187
13.6 Reading . . . 187
13.7 File manipulation again . . . 188
13.8 Reading using array sections . . . 189
13.9 Timing of reading formatted files . . . 190
13.10 Timing of reading unformatted files . . . 191
13.11 Errors when reading . . . 192
13.12 Summary . . . 193
13.13 Problems . . . 193

14 Files . . . 195
14.1 Data files in Fortran . . . 196
14.2 Summary of options on OPEN . . . 198
14.3 More foolproof I/O . . . 200
14.4 Summary . . . 201
14.5 Problems . . . 202

15 Functions . . . 204
15.1 An introduction to predefined functions and their use . . . 204
15.1.1 Example 1: Simple function usage . . . 205
15.2 Generic functions . . . 205
15.2.1 Example 2: The ABS generic function . . . 206
15.3 Elemental functions . . . 206
15.3.1 Example 3: Elemental function use . . . 206
15.4 Transformational functions . . . 206
15.4.1 Example 4: Simple transformational use . . . 207
15.4.2 Example 5: Intrinsic DOT_PRODUCT use . . . 207
15.5 Notes on function usage . . . 207
15.6 Example 6: Easter . . . 208
15.7 Complete list of predefined functions . . . 210
15.7.1 Inquiry functions . . . 210
15.7.2 Transfer and conversion functions . . . 210
15.7.3 Computational functions . . . 211
15.7.4 Array functions . . . 211
15.7.5 Predefined subroutines . . . 211
15.8 Supplying your own functions . . . 212
15.8.1 Example 7: Simple user defined function . . . 212
15.9 An introduction to the scope of variables and local variables . . . 214
15.10 Recursive functions . . . 214
15.10.1 Example 8: Recursive factorial evaluation . . . 215

15.11 Example 9: Recursive version of GCD . . . 216
15.12 Example 10: After removing recursion . . . 217
15.13 Pure functions . . . 218
15.14 Elemental functions . . . 218
15.15 Internal functions . . . 218
15.15.1 Example 11: Stirling's approximation . . . 218
15.16 Resumé . . . 219
15.17 Function syntax . . . 220
15.18 Rules and restrictions . . . 220
15.19 Problems . . . 220
15.20 Bibliography . . . 221
15.20.1 Recursion and problem solving . . . 222

16 Control Structures . . . 223
16.1 Selection among courses of action . . . 224
16.1.1 The BLOCK IF statement . . . 225
16.1.2 Example 1: Quadratic roots. . . . 227
16.1.3 Note . . . 228
16.1.4 Example 2: Date calculation . . . 228
16.1.5 The CASE statement. . . . 229
16.1.6 Example 3: Simple calculator. . . . 230
16.1.7 Example 4: Counting vowels, consonants, etc.. . . . 231
16.2 The three forms of the DO statement . . . 232
16.2.1 Example 5: Sentinel usage . . . 232
16.2.2 CYCLE and EXIT . . . 234
16.2.3 Example 6: e***x** evaluation . . . 234
16.2.4 Example 7: Wave breaking on an offshore reef . . . 235
16.3 Summary . . . 237
16.3.1 Control structure formal syntax . . . 237
16.4 Problems . . . 238
16.5 Bibliography . . . 240

17 Characters . . . 241
17.1 Character input . . . 243
17.2 Character operators . . . 244
17.3 Character substrings . . . 245
17.4 Character functions . . . 247
17.5 Collating sequence. . . . 248
17.6 Summary . . . 250
17.7 Problems . . . 251

18 Complex . . . 253
18.1 Example . . . 255
18.2 Complex and kind type . . . 256
18.3 Summary . . . 256

18.4 Problems . . . 256
19 Logical . . . 257
19.1 I/O . . . 261
19.2 Summary . . . 261
19.3 Problems . . . 262
20 User Defined Types . . . 263
20.1 Example 1: Dates . . . 264
20.2 Type definition . . . 264
20.3 Variable definition . . . 265
20.4 Example 2: Address lists . . . 265
20.5 Example 3: Nested user defined types . . . 266
20.6 Problems . . . 268
20.7 Bibliography . . . 268
21 An Introduction to Pointers . . . 269
21.1 Some basic pointer concepts . . . 270
21.2 The ASSOCIATED intrinsic function . . . 272
21.2.1 CVF 6.6C . . . 272
21.2.2 Intel, Windows, 8.1 . . . 272
21.2.3 Lahey, Windows 5.70f . . . 272
21.2.4 NAG, Windows, 4.2 . . . 273
21.2.5 Salford 4.6.0 . . . 273
21.3 Referencing A and B before assignment . . . 273
21.3.1 CVF . . . 274
21.3.2 Intel, Windows 8.1 . . . 274
21.3.3 Lahey, Windows 5.70f . . . 275
21.3.4 NAG, Windows 4.2 . . . 275
21.3.5 Salford 4.6.0 . . . 275
21.4 The NULL intrinsic . . . 275
21.5 Assignment via = . . . 276
21.6 Singly linked list . . . 278
21.7 Reading in an arbitrary quantity of numeric data . . . 280
21.8 Arrays of pointers . . . 283
21.9 Arrays of pointers and variable sized data sets — 1 . . . 284
21.10 Arrays of pointers and variable sized data sets — 2 . . . 285
21.11 Memory leak examples . . . 285
21.12 Nonstandard pointer examples . . . 288
21.13 Problems . . . 293
22 Introduction to Subroutines . . . 295
22.1 Example 1 . . . 296
22.1.1 Defining a subroutine . . . 298
22.1.2 Referencing a subroutine . . . 299

22.1.3 Dummy arguments or parameters and actual arguments 299
22.1.4 Intent 299
22.1.5 Local variables 299
22.1.6 Local variables and the SAVE attribute 300
22.1.7 Scope of variables 300
22.1.8 Status of the action carried out in the subroutine. 300
22.2 Example 2. 300
22.3 Example 3 — Quadratic example with interface blocks 301
22.4 Example 4 — Quadratic example and the CONTAINS statement. . 304
22.5 Why bother? 306
22.6 Summary 307
22.7 Problems 307
23 Subroutines: 2 309
23.1 More on parameter passing. 310
23.1.1 Explicit-shape array 310
23.1.2 Assumed-shape array 310
23.1.3 Deferred-shape array. 310
23.1.4 Automatic arrays 310
23.1.5 Assumed-size array — Fortran 77 style 310
23.1.6 Adjustable arrays — Fortran 77 style 311
23.2 Common code example 311
23.3 Explicit-shape example. 311
23.4 Assumed-shape example 313
23.4.1 Notes 315
23.5 Characters arguments and assumed-length dummy arguments . . . 315
23.6 Rank 2 and higher arrays as parameters 316
23.6.1 Explicit-shape dummy arrays. 316
23.6.2 Assumed-shape dummy array arguments 319
23.6.3 Notes 320
23.6.4 Using the intrinsic functions MATMUL and TRANSPOSE 321
23.7 Automatic arrays and median calculation 322
23.7.1 Internal subroutines and scope 325
23.7.2 Timing the selection sort algorithm 325
23.7.2.1 Timing 326
23.8 Alternative median calculation algorithm 327
23.8.1 Timing 330
23.9 Recursive subroutines — Quicksort. 332
23.9.1 Note — Interface blocks. 336
23.9.2 Note — Recursive subroutine 337
23.9.3 Note — Flexible design 337
23.9.4 Note — Timing information 337
23.10 Summary 337

23.11 Problems . . . 338
23.12 Bibliography . . . 340
23.13 Commercial numerical and statistical subroutine libraries . . . 340

24 An Introduction to Modules . . . 341
24.1 Modules for global data . . . 342
24.2 Modules for precision specification and constant definition. . . . 343
24.2.1 Note . . . 344
24.3 Modules for sharing arrays of data . . . 345
24.4 Modules for derived data types . . . 346
24.4.1 Person data type . . . 347
24.5 Modules containing procedures — Quicksort example . . . 349
24.6 Modules containing procedures — Statistics example . . . 353
24.7 The solution of linear equations using Gaussian elimination . . . 356
24.7.1 Notes . . . 361
24.7.1.1 Module for kind type . . . 361
24.7.1.2 Deferred-shape arrays . . . 361
24.7.1.3 Intrinisic functions MAXVAL and MAXLOC . . . 361
24.8 Notes on module usage and compilation . . . 361
24.9 Summary . . . 362
24.10 Problems . . . 362
24.11 Bibliography . . . 363

25 Converting from Fortran 77 . . . 365
25.1 Deleted features . . . 366
25.2 Obsolescent features . . . 366
25.2.1 Arithmetic IF . . . 366
25.2.2 Real and double precision DO control variables . . . 366
25.2.3 Shared DO termination and non-ENDDO termination . . . 366
25.2.4 Alternate RETURN . . . 367
25.2.5 PAUSE statement . . . 367
25.2.6 ASSIGN and assigned GOTO statements . . . 367
25.2.7 Assigned FORMAT statements . . . 367
25.2.8 H editing . . . 367
25.3 Better alternatives . . . 367
25.4 Example 1. . . . 368
25.5 Example 2. . . . 378
25.6 Commercial conversion tools . . . 379
25.6.1 NAG . . . 379
25.6.2 Polyhedron . . . 395
25.6.3 Original Fortran 66. . . . 407
25.6.4 Fortran 77 Version. . . . 407
25.6.5 Fortran 90 Version . . . 408
25.7 Summary . . . 409

25.8 Problems . . . 409
26 Case Studies . . . 411
26.1 Using linked lists for sparse matrix problems . . . 412
26.1.1 Inner product of two sparse vectors . . . 413
26.2 Solving a system of first-order ordinary differential equations using Runga–Kutta–Merson . . . 417
26.2.1 Note: Alternative form of the ALLOCATE statement . . . 424
26.2.2 Note: Automatic arrays . . . 424
26.2.3 Note: Dummy procedure arguments . . . 425
26.2.4 Keyword and optional arguments . . . 425
26.3 Generic procedures . . . 427
26.4 A function that returns a variable length array . . . 434
26.5 Operator and assignment overloading . . . 436
26.6 A subroutine to extract the diagonal elements of a matrix . . . 437
26.7 Perfectly balanced tree . . . 439
26.8 Pure function example . . . 442
26.8.1 Pure constraints . . . 442
26.9 Elemental function example . . . 443
26.9.1 Elemental constraints . . . 444
26.10 Elemental subroutine example . . . 445
26.11 Date class . . . 446
26.12 Graphics example — dislin . . . 461
26.13 Problems . . . 469
26.14 Bibliography . . . 470
27 ISO TR 15580 — IEEE Arithmetic . . . 473
27.1 History . . . 474
27.2 IEEE 754 Specifications . . . 476
27.2.1 Single precision floating point format . . . 477
27.2.2 Double precision floating point format . . . 479
27.2.3 Two classes of extended floating point formats . . . 479
27.2.4 Accuracy requirements . . . 479
27.2.5 Base conversion — Converting between decimal and binary floating point formats and vice versa . . . 479
27.2.6 Exception handling . . . 480
27.2.7 Rounding directions . . . 480
27.2.8 Rounding precisions . . . 480
27.3 Resumé . . . 480
27.4 ISO TR 15580 . . . 481
27.4.1 IEEE_FEATURES module . . . 481
27.4.2 IEEE_EXCEPTIONS module . . . 481
27.4.3 IEEE_ARITHMETIC module . . . 483
27.4.3.1 IEEE data type selection . . . 484

27.4.3.2 General support enquiry functions . . . 484
27.4.3.3 Rounding modes . . . 485
27.4.3.4 Number classification . . . 485
27.4.3.5 Arithmetic operations . . . 487
27.5 Summary . . . 488
27.6 Bibliography . . . 488
27.6.1 Web-based sources . . . 489
27.6.2 Hardware sources . . . 490
27.6.3 Operating Systems . . . 491
27.6.4 Java and IEEE 754 . . . 491
27.6.5 C and IEEE 754 . . . 492

28 ISO TR 15581 Allocatable Enhancements . . . 493
28.1 Allocatable dummy array example . . . 494
28.2 Allocatable function result example . . . 497
28.3 Allocatable structure component example . . . 499
28.4 Summary . . . 499
28.5 Problem . . . 499

29 Fortran 2003 and the Enhanced Module Facility . . . 501
29.1 Derived type enhancements . . . 502
29.2 Object oriented programming support . . . 502
29.3 Data manipulation enhancements . . . 502
29.4 Input/output enhancements . . . 503
29.5 Interoperability with the C programming language . . . 503
29.6 Procedure pointers . . . 504
29.7 Scoping enhancements . . . 504
29.8 Support for IEC 60559 (IEEE 754) exceptions and arithmetic . . . 504
29.9 Support for international usage: (ISO 10646) . . . 504
29.10 Enhanced integration with the host operating system . . . 505
29.11 The ASSOCIATE construct . . . 505
29.12 Enhanced modules facility . . . 505
29.13 Summary . . . 506

30 Parallel Programming . . . 507
30.1 MPI . . . 508
30.2 Co–array Fortran . . . 508
30.3 Openmp . . . 508
30.4 PVM . . . 509
30.5 HPF . . . 509
30.6 Parallel programming and high-performance computing . . . 509
30.6.1 Summary . . . 510

31 Miscellaneous . . . 511

31.1 Program development and software engineering . . . 512
31.1.1 Modules. . . . 513
31.1.2 Programming style — Programs should be easy to read . . . 513
31.1.3 Programming style — Programs should behave well . . . 514
31.2 Data structures. . . . 514
31.3 Algorithms . . . 514
31.4 Recursion . . . 515
31.5 Structured programming and the GOTO statement . . . 515
31.6 Efficiency, space-time trade-off. . . . 516
31.7 Program testing . . . 516
31.8 Simple debugging techniques . . . 516
31.9 Software tools . . . 517
31.9.1 Cross referencing . . . 517
31.9.2 Pretty print . . . 517
31.9.3 NAGWare f90 Tools . . . 517
31.10 Numerical software sources . . . 517
31.10.1 Numerical Algorithms Group . . . 518
31.10.2 Visual Numerics . . . 518
31.10.3 Netlib . . . 518
31.11 Coda . . . 518
31.12 Bibliography: All sources (bar one) taken from comp.software-eng. . . . 518
31.12.1 Software engineering. . . . 518
31.12.2 Programming style . . . 519
31.12.3 Software testing . . . 519
31.12.4 Fun . . . 519

A Glossary . . . 520

B Sample Program Examples. . . . 530

C ASCII Character Set . . . 534

D Intrinsic Functions and Procedures . . . 535

E English and Latin Texts . . . 568

F Coded Text Extract . . . 569

G Formal syntax . . . 570

H Compiler Options . . . 575

Index . . . 581

1

Overview

“I don't know what the language of the year 2000 will look like, but it will be called Fortran.”

C.A.R. Hoare

Aims

The aims of the chapter are to provide a background to the organisation of the book.

1 Overview

The book aims to provide coverage of a recommended subset of the full Fortran language. The subset we have chosen is one that fits most closely with the theory and practice of structured programming, data structuring and software engineering.

This book has been written for both complete beginners with little or no programming background and experienced Fortran programmers who want to update their skills and move to a modern version of the language.

Chapters 2–4 provide a short background to computer systems and their use:

- Chapter 2 looks at the basics of computer systems from the hardware point of view.
- Chapter 3 provides a short history of operating system developments and looks at some commonly used operating systems.
- Chapter 4 looks at some of the fundamentals of using a computer system.

These three chapters provide information that will be very helpful in the longer term for the successful use of computer systems for programming.

Chapters 5 and 6 provide a coverage of problem solving and the history and development of programming languages. Chapter 5 is essential for the beginner as the concepts introduced there are used and expanded on throughout the rest of the book. Chapter 6 must be read at some point but can be omitted initially. Programming languages evolve and some understanding of where Fortran has come from and where it is going will prove valuable in the longer term:

- Chapter 5 looks at problem solving in some depth, and there is a coverage of the way we define problems, the role of algorithms, the use of both top-down and bottom-up methods, and the requirement for formal systems analysis and design for more complex problems.
- Chapter 6 looks at the history and development of programming languages. This is essential as Fortran has evolved considerably from its origins in the mid-1950s, through the first standard in 1966, the Fortran 77 standard, the Fortran 90 standard, the Fortran 95 standard, TR 15580 and TR 15581, Fortran 2003 and beyond. It helps to put many of the current and proposed features of Fortran into context. Languages covered include Cobol, Algol, Lisp, Snobol, PL/1, Algol 68, Simula, Pascal, APL, Basic, C, Ada, Modula, Modula 2, Logo, Prolog, SQL, ICON, Oberon, Oberon 2, Smalltalk, C++, C# and Java.

Chapters 7 through 11 cover the major features provided in Fortran for numeric programming in the first instance and for general purpose programming in the sec-

ond. Each chapter has a set of problems. It is essential that a reasonable range of problems is attempted and completed, as it is impossible to learn any language without practice:

- Chapter 7 provides an introduction to programming with some simple Fortran examples. For people with a knowledge of programming this chapter can be covered fairly quickly.
- Chapter 8 looks at arithmetic in some depth, with a coverage of the various numeric data types, expressions and assignment of scalar variables. There is also a thorough coverage of the facilities provided in Fortran to help write programs that work on different hardware platforms.
- Chapter 9 is an introduction to arrays and DO loops. The chapter starts with some examples of tabular structures that one should be familiar with. There is then an examination of what concepts we need in a programming language to support manipulation of tabular data.
- Chapter 10 takes the ideas introduced in chapters 8 and 9 and extends them to higher-dimensioned arrays, additional forms of the DIMENSION attribute and corresponding form of the DO loop, and the use of looping for the control of repetition and manipulation of tabular information without the use of arrays.
- Chapter 11 looks at more of the facilities offered for the manipulation of whole arrays and array sections, ways in which we can initialise arrays using constructors, look more formally at the concepts we need to be able to accurately describe and understand arrays, and finally look at the differences between the way Fortran allows us to use arrays and the mathematical rules governing matrices.

Chapters 9 through 11 provide a coverage of some of the more important features and uses of arrays in the field of numerical problem solving. The framework provided here is drawn upon in later chapters in the book with more complex and realistic examples.

Chapters 12, 13 and 14 look at input and output (I/O) and file handling in Fortran. An understanding of I/O is necessary for the development of so-called production, non interactive programs. These are essentially fully developed programs that are used repeatedly with a variety of data inputs and results:

- Chapter 12 looks at output of results and how to generate something that is more comprehensible and easy to read than what is available with free format output and also how to write the results to a file rather than the screen.

- Chapter 13 extends the ideas introduced in Chapter 12 on output to cover input of data, or reading data into a program and also considers file I/O.
- Chapter 14 provides a coverage of files.

Chapter 15 introduces the first building block available in Fortran for the construction of programs for the solution of larger, more complex problems. It looks at the functions available in Fortran, the so-called intrinsic functions and procedures (over 100 of them) and covers how you can define and use your own functions.

It is essential to develop an understanding of the functions provided by the language and when it is necessary to write your own.

Chapter 16 introduces more formally the concept of control structures and their role in structured programming. Some of the control structures available in Fortran are introduced in earlier chapters, but there is a summary here of those already covered plus several new ones that complete our coverage of a minimal working set.

Chapters 17 through 21 complete our coverage of the facilities for data typing and structuring provided by Fortran, both predefined and user defined. Fortran has now caught up with some of the major developments in the data-structuring area of the last 20 years, which have been available in other languages for some time:

- Chapter 17 looks at the character data type in Fortran. There is a coverage of I/O again, with the operators available — only one in fact.
- Chapter 18 looks at the last numeric data type in Fortran, the complex data type. This data type is essential to the solution of a small class of problems in mathematics and engineering.
- Chapter 19 looks at the logical data type. The material covered here helps considerably in increasing the power and sophistication of the way we use and construct logical expressions in Fortran. This proves invaluable in the construction and use of logical expressions in control structures.
- Chapters 20 looks at user-defined data types. This introduces another major new feature of Fortran. Previous versions of the language lacked any facilities in this area. This meant that in many applications earlier versions of Fortran were not the language of first choice for many people.
- Chapter 21 looks at the dynamic data-structuring facilities now available in Fortran. Examples are drawn from a range of sources.

These chapters conclude coverage of the data-structuring facilities provided by Fortran. There are problems that will require facilities not provided, but it is surprising what can be achieved with the set now provided in Fortran. The material

covered is extended into more realistic examples when we look at the construction of larger and more complex programs in the last few chapters in the book.

The next two chapters look at the second major building block in Fortran — the subroutine. Chapter 22 provides a gentle introduction to some of the fundamental concepts of subroutine definition and use and Chapter 23 extends these ideas.

Chapter 24 introduces the concept of a module and the range of things that it brings to Fortran.

Chapter 25 looks at converting to modern Fortran. A number of examples are used and several software tools are examined.

Chapter 26 has a number of case studies helping to pull together the ideas presented in the earlier chapters.

Chapter 27 looks at ISO TR 15580 — IEEE Arithmetic.

Chapter 28 deals with ISO TR 15581 — Allocatable Enhancements

Chapters 29 covers the new features of Fortran 2003 and ISO/IEC DTR 19767, Enhanced Module Facilities.

Chapter 30 examines parallel Fortran.

Chapter 31 ties up some loose ends. It looks at program development and software engineering, modules, programming style, data structures, algorithms, structured programming, recursion and recursion removal, efficiency in space and time, program testing, simple debugging techniques, software tools and numerical software sources. There is also coverage of the various internet resources available for Fortran.

Many of the chapters have annotated bibliographies. These often have pointers and directions for further reading. The coverage provided cannot be seen in isolation. The concepts introduced are by intention brief, and fuller coverage must be sought where necessary.

There are several appendices:

- Appendix A — This is a glossary which provides coverage of both the new concepts provided by Fortran and a range of computing terms and ideas.
- Appendix B — Provides an example of a simple program in a number of the languages described in the chapter on program language development. There is also coverage of the standards that apply.
- Appendix C — The ASCII character set.

- Appendix D — Contains a list of all of the intrinsic procedures in Fortran and includes a full explanation of each procedure with a coverage of the rules and restrictions that apply and examples of use.
- Appendix E — Contains the English and Latin text extracts used in one of the problems in the chapter on characters.
- Appendix F — Contains the coded text extract used in one of the problems in Chapter 17.
- Appendix G — Formal syntax
- Appendix H — Sample compiler options

This book is not and cannot possibly be completely self-contained and exhaustive in its coverage of the Fortran language. Our first intention has been to produce a coverage of the features that will get you started with Fortran and enable you to solve quite a wide range of problems successfully.

Fortran, like most languages, has features that are of relatively little use or make the construction of larger-scale programs more difficult, especially when moving between hardware platforms. We have deliberately avoided these features.

Another problem is backwards compatibility with Fortran 77. Existing Fortran 77 programs have to be maintained, and there is much in that language that is *deprecated* or *obsolescent* in terms of Fortran 95 and Fortran 2003.

We have aimed to introduce a working subset of the new language that emphasises the better constructs provided in Fortran over its predecessors, Fortran 77 and Fortran 66.

All in all Fortran is an exciting language, and it has *caught up* with language developments of the 1970s, 1980s, and 1990s.

A range of hardware platforms, operating systems and Fortran compilers were used. These include:

- DEC VAX under VMS and later Open VMS using the NAG Fortran 90 compiler.
- DEC Alpha under Open VMS using the DEC/Compaq Fortran 90 compiler.
- PC under DOS and Windows, DEC/Compaq Fortran 90.
- PC under DOS and Windows, DEC/Compaq/HP Fortran 95.
- PC under DOS and Windows, NAG/Salford Fortran 90.
- PC under DOS and Windows, Lahey Fujitsu Fortran 95 PRO 5.7.

- PC under DOS and Windows, Intel.
- PC under DOS and Windows, NAGWare f95.
- Sun UltraSparc under Solaris using NAGWare F90.
- Sun UltraSparc under Solaris using NAGACE F90.
- Sun UltraSparc under Solaris using NAGWare F95.
- Sun UltraSparc under Solaris using Sun F90.
- Intel Linux, NAGWare f95.
- Intel Linux, Lahey Fujitsu Fortran 95 PRO, 6.1.
- Intel Linux, Intel.

Our recommendation is that you use at least two compilers in the development of your code. Moving code between platforms teaches you a lot.

We are the current owners of the Fortran 90 list, and quoting the introduction "*This list covers all aspects of Fortran 90 and HPF, the new standard(s) for Fortran. The emphasis should be on the *new* features of Fortran 90. It welcomes contributions from people who write Fortran 90 applications, teach it in courses, want to port programs and use it on (super)computers.*"

Visit:

- http://www.jiscmail.ac.uk/lists/comp-fortran-90.html

for more information.

Ian Chivers is also Editor of Fortran Forum, the SIGPLAN Special Interest Publication on Fortran, ACM Press.

2

Introduction to Computer Systems

"Don't Panic."

Douglas Adams, *The Hitch Hiker's Guide to the Galaxy*

Aims

The aims of this chapter are to introduce the following:

- The components of a computer — the hardware.
- The components of a complete computer system — the other devices that you need to do useful work with a computer.
- The software needed to make the hardware do what you want it do.

2 Introduction to Computer Systems

A computer is an electronic device and can be thought of as a tool like a lever or a wheel, which can be made to do useful work. At the fundamental level it works with *bits* (binary digits or sequences of zeros and ones). Bits are generally put together in larger configurations, e.g., 8, 16, 32, or 64. Hence computers are often referred to as 8-bit, 16-bit, 32-bit, or 64-bit machines.

2.1 The core of a computer system

The heart of most computer systems comprises a motherboard, CPU, memory, one or more busses and a power supply. We will look at the CPU, memory and bus in more depth below.

2.1.1 Central processor unit — CPU

This is the brains of the computer. All of the work that the computer does is organised here.

2.1.2 Memory

The computer also has a memory. Memory on a computer is a solid state device that comprises an ordered collection of bits/bytes/words that can be read or written by the CPU. A byte is generally 8 bits (as in *8-bit byte*), and a word is most commonly accepted as the minimum number of bits that can be referenced by the CPU. This referencing is called *addressing*. The memory typically contains programs and data.

The two most common word sizes are 32 and 64 bits.

A computer memory is often called random access memory, or RAM. This simply means that the access time for any part of the memory is the same; in order to examine location (say) 97, it is not necessary to first look through locations 1 to 96. It is possible to go directly to location 97. A slightly better term might have been *access at random*. The memory itself is highly ordered.

2.1.3 Bus

A *bus* is a set of connections between the CPU and other components. The bus is used for a variety of purposes. These include address signals, which tell the memory which words are wanted next and data lines, which are used to transfer data to and from memory and to and from other parts of the computer system. This is typical of many systems, but systems do vary considerably; so while the information above may not be true in specific cases, it provides a general model.

2.2 Other components of a computer system

So far the computer we have described is not sufficiently versatile. We have to add on other pieces of electronics to make it really useful.

2.2.1 Disks

These are devices for storing collections of *bits*, which are inevitably organised in reality into bytes and files. One advantage of adding these to our computer system is that we can switch the machine off, go away and come back at a later time and continue with what we were doing.

Memory is expensive and fast, whereas disks are slower but cheaper. Most computer systems balance speed against cost, and have a small memory in relation to disk capacity.

Many people will be familiar with the two main types of disks on early personal computers (PCs) or microcomputers: floppy disks and hard disks. Floppy disks now come in one main physical size, 3-1/2 inch, but smaller ones are also used. Hard disks are inside the system, and most people do not see them.

Optical drives are an essential part of present day systems. They exist in a variety of flavours including simple read-only CD, rewritable CD and DVD forms.

2.2.2 Others

There are a large number of other input and output devices. These vary considerably from system to system, depending on the work being carried out. They include:

- Network (ethernet or wifi) cards for access to local and wide area networks.
- Modems for access from home, mainly to the Internet.
- Printers of a variety of types.
- Colour plotters.
- Phototypesetters.
- Pens.
- Sound interfaces, both for speech recognition and sound production.
- Scanners.
- Digital cameras.
- Joy sticks.
- Zip drives.

- Memory sticks.

The most important I/O devices are the keyboard and the screen, whether you use a terminal, PC or workstation. This book has been written assuming that most of your work will be done at one of these devices.

Terminals fall into two categories, character-based devices (and the DEC VT series is a very popular one) and graphical devices (the X-Windows terminals are the most popular). Terminal access to remote systems is often provided on PCs using terminal emulation software, e.g., Telnet, WinQVT and X-Windows access to UNIX systems via software like Vista Exceed.

PCs provide the opportunity for cheap and powerful desktop computing facilities, where the processing is done locally.

Workstations are more powerful than microcomputers but this division is becoming rather blurred with the recent generations of processors. Screens on these devices are graphically oriented. Access to these systems is via a graphical or windows interface.

This means that the device we use looks rather like an ordinary typewriter keyboard, although some of the keys are different. However, the location of the letters, numbers and common symbols is fairly standard. Don't panic if you have never met a keyboard before. You don't have to know much more than where the keys are. Few programmers, even professionals, advance beyond the stage of using two index fingers and a thumb for typing. You will find that speed in typing is rarely important; it's accuracy that counts.

One thing that people unfamiliar with keyboards often fail to realise is that what you have typed in is not sent to the computer until you press the *carriage return* key. To achieve any sort of communication you must press that key; it will be somewhere on the right-hand side of the keyboard, and will be marked *return, c/r, send, enter*, or something similar.

2.3 Software

So far we have not mentioned software. Software is the name given to the programs that *run* on the hardware. Programs are written in *languages.* Computer languages are frequently divided into two categories: *high level* and *low level.* A low-level language (e.g., assembler) is closer to the hardware, whereas a high-level language (e.g., Fortran) is closer to the problem statement. There is typically a one-to-one correspondence between an assembly language statement and the actual hardware instruction. With a high-level language there is a one-to-many correspondence; one high-level statement will generate many machine-level instructions.

A certain amount of general purpose software will have been provided by the manufacturer. This software will typically include the basic operating system, one or more *compilers*, an *assembler*, an *editor*, and a *loader* or *link editor*.

- A *compiler* translates high-level statements into machine instructions.
- An *assembler* translates low-level or assembly language statements into machine instructions.
- An *editor* makes changes to text files, e.g., program sources.
- A *loader* or *link editor* takes the output from the compiler and completes the process of generating something that can be executed on the hardware.

These programs will vary considerably in size and complexity. Certain programs that make up the operating system will be quite simple and small (like copying utilities), whereas certain others will be relatively large and complex (like a compiler).

In this book we concentrate on software or programs that you write for your research or course work. As the book progresses you will be introduced to ways of building on what other people have produced and how to take advantage of the vast amount of software already written, tested and documented.

2.4 Problems

1. Distinguish between a memory address and memory contents.

2. What does RAM stand for?

3. What would a WOM (write only memory) do? How would you use it?

4. What does CPU stand for? What does it do?

5 What does a compiler do?

6 What does a linker do?

2.5 Bibliography

Baer J.L., *Computer Systems Architecture*, Computer Science Press.

Extremely readable coverage of this whole area. The version could do with an update, but it is still a very impressive coverage. Highly recommended.

Bhandarkar D.P., *Alpha Implementation and Architecture: Complete Reference and Guide*, Digital Press, 1996.

Excellent source of information on the Alpha architecture.

Intel currently make a lot of material available on their web site. Two useful URLs are:

- http://www.intel.com/

and

- http://developer.intel.com/

Well worth a look. Many publications are available in Adobe Acrobat Portable Document Format — PDF.

Reeves C.M., *An Introduction to Logical Design of Digital Circuits*, CUP, 1972.

This book provides coverage of the construction of the very simple electronic building blocks from which most modern computer systems are made. Relatively theoretical.

Tannenbaum A.S., *Structured Computer Organisation*, Prentice-Hall, 1976.

Very good coverage looking at a computer system in terms of a hierarchy of levels. An easy read.

3

Introduction to Operating Systems

"'Where shall I begin your Majesty' he asked.
'Begin at the beginning,' the King said, gravely 'and go on till you come to the end then stop.'"

Lewis Carroll, *Alice's Adventures in Wonderland*

Aims

The aims of this chapter are:

- To provide a brief history of operating system development.
- To look briefly at some commonly used operating systems:
  - DOS and Windows.
  - UNIX and X-Windows.
  - Linux and X-Windows.
  - VMS and Open VMS.

3 Introduction to Operating Systems

A simple definition of an operating system is the suite of programs that make the hardware usable. Most computer systems provide one. They vary considerably from those available on early microcomputers, like CP/M, to DOS and the various versions of Microsoft Windows on PCs and UNIX with X-Windows and Linux with X-Windows on workstations and supercomputers.

From the designer's point of view operating systems are mainly resource managers. They allow management of the CPU, disks and I/O devices. They have to provide a user interface for computer operators, professional programmers (whether systems or applications), administrators of the system, and finally the casual end user. As can be imagined, these groups have different functional requirements. It is therefore useful to look at the development of operating systems, and see a shift from satisfying the requirements of the professional to satisfying the requirements of the casual end user.

3.1 History of operating systems

3.1.1 The 1940s

Early computer systems had no operating systems in the modern sense of the word. An early commercially available machine was the IBM 604 which could undertake some 60 program steps before using punch cards as backing store. The end user had intimate knowledge of the machine and programmed at a very low level.

3.1.2 The 1950s

This era saw a rapid change in the capabilities of operating systems. They were designed to make efficient use of an expensive resource. Jobs were *batched* so that the time between jobs was minimised. The end user was now distanced from the machine. This era saw rapid development in program language design and a notable end to the period was the design of Algol 60.

3.1.3 The 1960s

The next milestone was the introduction of multiprogramming. Probably initially seen as a way of making efficient use of hardware it heralded the idea of time sharing. A time-sharing system is characterised by the conversational nature of the interaction and the use of a keyboard. This had a tremendous impact on the range of uses that a computer system had and on the program development process.

3.1.4 The 1960s and 1970s

The realisation that computer systems could be used in a wide range of human activities saw the development of large, general purpose systems, and probably the most famous of these was the IBM 360 series. These systems were some of the

most complex programming endeavours undertaken, and most projects were late and well over budget. These costly mistakes helped lead to the establishment of software engineering as a discipline.

The contribution of the time-sharing system to program development was quickly realised to be considerable. A system that was developed during this period was UNIX — and this operating system has a very sharp set of tools to aid in program development.

3.1.5 The 1970s, 1980s, and 1990s

The 1970s represented a period of relative stability with newer and more complex versions of existing systems.

During this period the importance of graphical interfaces emerged and, with dropping hardware costs, graphical interfaces started to dominate.

The Apple Macintosh heralded a new era and became a popular choice for many people. At the same time graphical interfaces were being added to existing major operating systems, with X-Windows and associated higher-level systems hiding raw UNIX from many users and Microsoft Windows on the Intel family of processors.

Linux (a free UNIX variant) is popular in the scientific field, and a very good alternative to DOS and Windows on the Intel family of processors.

3.2 Networking

Networking simplistically is a way of connecting two or more computer systems. Networking computer systems is not new. One of the first was the SAGE military network, funded by the US DoD in the 1950s.

Networking capability has undergone a massive increase during the computer age. Local networks of two or three systems through tens of systems in small research groups and organizations are now extremely common place. It is not unusual now to have in excess of a thousand network connected devices on one local area network.

Wide-area networking is also quite common, and most major organisations now have networks spanning a country or even the whole world.

One of the most widely used wide-area networks in the academic and scientific world is the Internet, and there are many millions of systems on the Internet at the time of writing this book.

A number of books on networking are included in the bibliography.

3.3 Problems

1. What type of system do you use, i.e., is it a stand alone microcomputer, terminal, workstation, etc?

2. Is it networked, and if so in what way?

3. Is wide-area networking available?

4. Is a graphical interface available?

3.4 Bibliography

Brooks F.P., *The Mythical Man Month: Essays on Software Engineering,* Addison-Wesley, 1982.

A very telling coverage of the development of the operating system for the IBM 360 series of systems. A must for any one involved in the longer term in program development.

Deitel H.M., *An Introduction to Operating Systems*, Addison-Wesley, 1984.

One of the most accessible books on operating systems with coverage of process management, storage management, processor management, auxiliary storage management, performance, networks and security, with case studies of the major players including UNIX, VMS, CP/M, MVS, VM, DOS and Windows.

Feit S., *TCP/IP, Architecture, Protocols, and Implementation,* McGraw-Hill.

A more technical book than Kroll, well written with a wealth of information for the more inquisitive reader.

Kroll E., *The Whole Internet User's Guide and Catalog,* O'Reilly, 1994.

The Internet book. Written with very obvious enthusiasm by Mister Internet himself!

4

Introduction to Using a Computer System

"Maybe one day we will be glad to remember even these things."

Virgil

Aims

The aims of this chapter are to introduce some of the fundamentals of using a computer system, including:

- Files.
- Editors.
- Systems access and networking.

4 Introduction to Using a Computer System

There are a number of concepts that underpin your use of any computing system. Sitting at a high-resolution colour screen with a myriad of icons this may not be immediately apparent, but developing an appreciation of it will help considerably in the long term and when you inevitably move from one system to another.

4.1 Files

A file is a collection of information that you refer to by name, e.g., if you were to use a word processor to prepare a letter then the letter would exist independently as a file on that system, generally on a disk. With graphical interfaces there will be a systematic iconic representation of files.

There will be many ways of manipulating files on the operating system that you work on. You will use an editor to make changes to a file. This file might be the source of a program and you could then use a compiler to compile your program. The compiler will generate a number of files, some of interest to you, others for its own use. There will be commands in the operating system to make copies of files, back files up onto a variety of media, etc.

4.2 Editors

All general purpose computer systems have at least one editor so that you can modify programs and data. Screen editors are by far the easiest to use, with changes you make to the file being immediately visible on the screen in front of you.

Some editors will have sophisticated command modes of operation with pattern matching allowing very powerful text-processing capabilities. These can automate many common tasks, taking away the manual, repetitive drudgery of screen-based editing.

4.3 Single-user systems

These are becoming increasingly common, in use both at work and in the home. The PC is a very popular choice in the scientific community. They offer ease of use and access to a considerable amount of raw processing power for computer-intensive applications.

4.4 Networked systems

It is quite common to interconnect the above to local and wide-area networks. This same network would also have file servers, printers, plotters, mail gateways, etc. Both authors have PCs with modems at home and have access via the telephone system to the Internet.

Workstations are generally networked in an environment like the above, providing very powerful processing capability.

4.5 Multiuser systems

One step above microcomputers and workstations are multiuser systems. The dividing lines between microcomputers, individual workstations and multiuser systems are rapidly becoming blurred.

Multiuser systems, especially the larger ones, are very popular as they relieve the casual end users from much of the drudgery of the day-to-day tasks: backing up disks, installing new versions of the software, locating and fixing problems with software that doesn't work quite as it should, etc., are carried out by a system manager or operator.

Here we find one person with the role of registering new users, backing up the file system, sorting out printer problems, networking problems, etc. This also means that not all of the users of the system have to remember rather arcane and sometimes rather magical commands! They can get on with solving their actual problems.

4.6 Other useful things to know

You will soon need to know what files you are working with and there will be commands to do this. There will be a need to get rid of files and there will be commands to achieve this.

There will be ways of getting on-line help, and *help* as a command is (for once!) used by a variety of operating systems. On UNIX systems the rather more unintelligible *man* command is available.

There will be commands to print program listings and data files

With networked and multiuser systems there will be commands to send and receive electronic mail to/from other users. It is easy to send and reply to mail from people across the world, often in hours and even minutes. Table 4.1 has examples of some common operating system commands in DOS, UNIX, Linux and VMS.

Operating system and command	DOS	UNIX Linux	VMS
What files are there	dir	ls	dir
Get rid of a file	del	rm	del
Copy a file	copy	cp	copy
Display a file on the screen	type	cat	type
Print a file	print	pr	print
Create or make changes to a file	edit	ed	edit
		vi	edit/tpu
Make a subdirectory	mkdir, md	md	create/dir
Change to another directory	chdir, cd	cd	set default

Table 4.1 Common Operating System Commands

4.7 Common methods of using computer systems to develop Fortran programs

The following are some of the ways in which you can use a computer system to develop Fortran programs:

- PC running Windows and X-Windowing software to access a remote system with a Fortran compiler installed, GUI interface.
- PC running Linux and X-Windows to access a remote system with a Fortran compiler installed, GUI interface.
- PC running Windows and telnet or ssh to access a remote system with a Fortran compiler installed, terminal-style interface.
- PC running Linux and telnet or ssh to access a remote system with a Fortran compiler installed, terminal-style interface.
- PC running Windows, local Fortran compiler installed.
- PC running Linux, local Fortran compiler installed.
- Proprietary workstation, local compiler installed.
- Proprietary workstation, accessing compiler on remote system.

All will have one thing in common and that is that the following cycle is used:

- Edit your program.
- Compile the program.
- Run the program.
- Check the answers.
- Go back and edit the program to correct the errors and repeat until the answers are what you expect!

4.8 Bibliography

The main sources here are the manuals and documentation provided by the supplier of whatever system you use. These are increasingly of a very high standard. However they are inevitably written to highlight the positive and downplay the negative aspects of the systems. The next sources are the many third-party books written and widely available throughout the world. These vary considerably in price from basic introductory coverages to very comprehensive reference works. These are a very good complement to the first. The following URL is a very good source of UNIX information.

- http://unixhelp.ed.ac.uk/

Gilly D., *UNIX in a Nutshell,* O'Reilly.

A very good quick reference guide. Assumes some familiarity with UNIX. Current edition (at the time of writing this book) was System V Release IV, with Solaris 2.0. Also provides coverage of the various shells, Bourne, Korn and C.

Microsoft, *Windows User's Guide*, Microsoft Press.

Good coverage of Windows and suitable for the beginner and intermediate level user. Sufficient for most users. A massive improvement over earlier versions.

5

Introduction to Problem Solving

"They constructed ladders to reach to the top of the enemy's wall, and they did this by calculating the height of the wall from the number of layers of bricks at a point which was facing in their direction and had not been plastered. The layers were counted by a lot of people at the same time, and though some were likely to get the figure wrong the majority would get it right... Thus, guessing what the thickness of a single brick was, they calculated how long their ladder would have to be."

Thucydides, *The Peloponnesian War*

"'When I use a word,' Humpty Dumpty said, in a rather scornful tone, 'it means just what I choose it to mean — neither more nor less.'
'The question is,' said Alice, 'whether you can make words mean so many different things.'"

Lewis Carroll, *Through the Looking Glass and What Alice Found There*

Aims

The aims of this chapter are:

- To examine some of the ideas and concepts involved in problem solving.
- To introduce the concept of an algorithm.
- To introduce two ways of approaching algorithmic problem solving.
- To introduce the ideas involved with systems analysis and design, i.e., to show the need for pencil and paper study before using a computer system.

5 Introduction to Problem Solving

It is informative to consider some of the dictionary definitions of problem:

- A matter difficult of settlement or solution, *Chambers*.
- A question or puzzle propounded for solution, *Chambers*.
- A source of perplexity, *Chambers*.
- Doubtful or difficult question, *Oxford*.
- Proposition in which something has to be done, *Oxford*.
- A question raised for enquiry, consideration, or solution, *Webster's*.
- An intricate unsettled question, *Webster's*.

A common thread seems to be a question that we would like answered or solved. So one of the first things to consider in problem solving is how to pose the problem. This is often not as easy as is seems. Two of the most common methods to use here are:

- In natural language.
- In artificial or stylised language.

Both methods have their advantages and disadvantages.

5.1 Natural language

Most people use natural language and are familiar with it, and the two most common forms are the written and spoken word. Consider the following language usage:

- The difference between a 3-year-old child and an adult describing the world.
- The difference between the way an engineer and a physicist would approach the design of a car engine.
- The difference between a manager and a worker considering the implications of the introduction of new technology.

Great care must be taken when using natural language to define a problem and a solution. It is possible that people use the same language to mean completely different things, and one must be aware of this when using natural language whilst problem solving.

Natural language can also be ambiguous: Old men and women eat cheese. Are both the men and women old?

5.2 Artificial language

The two most common forms of artificial language are technical terminology and notations. Technical terminology generally includes both the use of new words and alternate use of existing words. Consider some of the concepts that are useful when examining the expansion of gases in both a theoretical and practical fashion:

- Temperature.
- Pressure.
- Mass.
- Isothermal expansion.
- Adiabatic expansion.

Now look at the following:

- A chef using a pressure cooker.
- A garage mechanic working on a car engine.
- A doctor monitoring blood pressure.
- An engineer designing a gas turbine.

Each has a particular problem to solve, and all will approach their problem in their own way; thus they will each use the same terminology in slightly different ways.

5.2.1 Notations

Some examples of notations are:

- Algebra.
- Calculus.
- Logic.

All of the above have been used as notations for describing both problems and their solutions.

5.3 Resumé

We therefore have two ways of describing problems and they both have a learning phase until we achieve sufficient understanding to use them effectively. Having arrived at a satisfactory problem statement we next have to consider how we get the solution. It is here that the power of the algorithmic approach becomes useful.

5.4 Algorithms

An algorithm is a sequence of steps that will solve part or all of a problem. One of the most easily understood examples of an algorithm is a recipe. Most people have done some cooking, if only making toast and boiling an egg.

A recipe is made up of two parts:

- A check list of things you need.
- The sequence or order of steps.

Problems can occur at both stages, e.g., finding out halfway through the recipe that you do not have an ingredient or utensil; finding out that one stage will take an hour when the rest will be ready in ten minutes. Note that certain things can be done in any order — it may not make any difference if you prepare the potatoes before the carrots.

There are two ways of approaching problem solving when using a computer. They both involve *algorithms*, but are very different from one another. They are called *top-down* and *bottom-up.*

5.4.1 Top-down

In a *top-down* approach the problem is first specified at a high or general level: prepare a meal. It is then refined until each step in the solution is explicit and in the correct sequence, e.g., peel and slice the onions, then brown in a frying pan before adding the beef. One drawback to this approach is that it is very difficult to teach to beginners because they rarely have any idea of what *primitive* tools they have at their disposal. Another drawback is that they often get the sequencing wrong, e.g., *now place in a moderately hot oven* is frustrating because you may not have lit the oven (sequencing problem) and secondly because you may have no idea how hot *moderately hot* really is. However, as more and more problems are tackled, top-down becomes one of the most effective methods for programming.

5.4.2 Bottom-up

Bottom-up is the reverse to top-down! As before you start by defining the problem at a high level, e.g., prepare a meal. However, now there is an examination of what tools, etc. you have available to solve the problem. This method lends itself to teaching since a repertoire of tools can be built up and more complicated problems can be tackled. Thinking back to the recipe there is not much point in trying to cook a six course meal if the only thing that you can do is boil an egg and open a tin of beans. The bottom-up approach thus has advantages for the beginner. However, there may be a problem when no suitable tool is available. A colleague and friend of the authors learned how to make Bechamel sauce, and was so pleased by his success that every other meal had a course with a Bechamel sauce. Try it on

your eggs one morning. Here is a case of specifying a problem, *prepare a meal*, and using an inappropriate but plausible tool, *Bechamel sauce.*

The effort involved in tackling a realistic problem, introducing the constructs as and when they are needed and solving it is considerable. This approach may not lead to a reasonably comprehensive coverage of the language, or be particularly useful from a teaching point of view. Case studies do have great value, but it helps if you know the elementary rules before you start on them. Imagine learning French by studying Balzac, before you even look at a French grammar book. You can learn this way but even when you have finished, you may not be able to speak to a Frenchman and be understood. A good example of the case study approach is given in the book *Software Tools*, by Kernighan and Plauger.

In this book our aim is to gradually introduce more and more tools until you know enough to approach the problem using the top-down method, and also realise from time to time that it will be necessary to develop some new tools.

5.4.3 Stepwise refinement

Both of the above techniques can be combined with what is called *stepwise refinement*. The original ideas behind this approach are well expressed in a paper by Wirth, entitled "Program Development by Stepwise Refinement", published in 1971. It means that you start with a global problem statement and break the problem down in stages, into smaller and smaller subproblems that become more and more amenable to solution. When you first start programming the problems you can solve are quite simple, but as your experience grows you will find that you can handle more complex problems.

When you think of the way that you solve problems you will probably realise that unless the problem is so simple that you can answer it straightaway some thinking and pencil and paper work are required. An example that some may be familiar with is in practical work in a scientific discipline, where coming unprepared to the situation can be very frustrating and unrewarding. It is therefore appropriate to look at ways of doing analysis and design before using a computer.

5.4.4 Modular programming

As the problems we try solving become more complex we need to look at ways of managing the construction of programs that comprise many parts. Modula 2 was one of the first languages to support this methodology and we will look at modular programming in more depth in a subsequent chapter.

5.4.5 Object oriented programming

There is a class of problems that are best solved by the treatment of the components of these problems as objects. We will look at the concepts involved in object oriented programming and object oriented languages in the next chapter.

5.5 Systems analysis and design

When one starts programming it is generally not apparent that one needs a methodology to follow to become successful as a programmer. This is usually because the problems are reasonably simple, and it is not necessary to be explicit about all of the stages one has gone through in arriving at a solution. As the problems become more complex it is necessary to become more rigorous and thorough in one's approach, to keep control in the face of the increasing complexity and to avoid making mistakes. It is then that the benefit of systems analysis and design becomes obvious. Broadly we have the following stages in systems analysis and design:

- Problem definition.
- Feasibility study and fact finding.
- Analysis.
- Initial system design.
- Detailed design.
- Implementation.
- Evaluation.
- Maintenance.

and each problem we address will entail slightly different time spent in each of these stages. Let us look at each stage in more detail.

5.5.1 Problem definition

Here we are interested in defining what the problem really is. We should aim at providing some restriction on both the scope of the problem, and the objectives we set ourselves. We can use the methods mentioned earlier to help us out. It is essential that the objectives are:

- Clearly defined.
- Understood and agreed to by all people concerned, when more than one person is involved.
- Realistic.

5.5.2 Feasibility study and fact finding

Here we look to see if there is a feasible solution. We would try and estimate the cost of solving the problem and see if the investment was warranted by the benefits, i.e., cost-benefit analysis.

5.5.3 Analysis

Here we look at what must be done to solve the problem. Note that we are interested in finding out what we need to do, but that we do not actually do it at this stage.

5.5.4 Design

Once the analysis is complete we know what must be done, and we can proceed to the design. We may find there are several alternatives, and we thus examine alternate ways in which the problem can be solved. It is here that we use the techniques of top-down and bottom-up problem solving, combined with stepwise refinement to generate an algorithm to solve the problem. We are now moving from the logical to the physical side of the solution. This stage ends with a choice among several alternatives. Note that there is generally not one ideal solution, but several, each with its own advantages and disadvantages.

5.5.5 Detailed design

Here we move from the general to the specific, The end result of this stage should be a specification that is sufficiently tightly defined specification to generate actual program code.

It is at this stage that it is useful to generate *pseudocode*. This means writing out in detail the actions we want carried out at each stage of our overall algorithm. We gradually expand each stage (stepwise refinement) until it becomes Fortran — or whatever language we want.

5.5.6 Implementation

It is at this stage that we actually use a computer system to create the program(s) that will solve the problem. It is here that we actually need to know enough about a programming language to use it effectively to solve our problem. This is only one stage in the overall process, and mistakes at any of the stages can create serious difficulties.

5.5.7 Evaluation and testing

Here we try to see if the program(s) we have produced will actually do what they are supposed to. We need to have data sets that enable us to say with confidence that the program really does work. This may not be an easy task, as quite often we only have numeric methods to solve the problem, which is why we are using the computer in the first place — hence we are relying on the computer to provide the proof; i.e., we have to use a computer to determine the veracity of the programs — and as Heller says, *Catch 22.*

5.5.8 Maintenance

It is rare that a program is run once and never used again. This means that there will be an ongoing task of maintaining the program, generally to make it work with different versions of the operating system or compiler, and to incorporate new features not included in the original design. It often seems odd when one starts programming that a program will need maintenance, as we are reluctant to regard a program in the same way as a mechanical object like a car that will eventually fall apart through use. Thus maintenance means keeping the program working at some tolerable level, often with a high level of investment in manpower and resources. Research in this area has shown that anything up to 80% of the manpower investment in a program can be in maintenance.

5.6 Conclusions

A drawback, inherent in all approaches to programming and to problem solving in general, is the assumption that a solution is indeed possible. There are problems which are simply insoluble — not only problems like balancing a national budget, weather forecasting for a year, or predicting which radioactive atom will decay, but also problems which are apparently computationally solvable.

Knuth gives the example of a chess problem — determining whether the game is a forced victory for white. Although there is an algorithm to achieve this, it requires an inordinately long time to complete. For practical purposes it is unsolvable.

Other problems can be shown mathematically to be undecidable. The work of Gödel in this area has been of enormous importance, and the bibliography contains a number of references for the more inquisitive and mathematically orientated reader. The Hofstader coverage is the easiest, and least mathematical.

As far as possible we will restrict ourselves to solvable problems, like learning a programming language.

Within the formal world of Computer Science our description of an algorithm would be considered a little lax. For our introductory needs it is sufficient, but a more rigorous approach is given by Hopcroft and Ullman in *Introduction to Automata Theory, Languages and Computation*, and by Beckman in *Mathematical Foundations of Programming.*

5.7 Problems

1. What is an algorithm?

2. What distinguishes top-down from bottom-up approaches to problem solving? Illustrate your answer with reference to the problem of a car, motor-cycle or bicycle having a flat tire.

5.8 Bibliography

Aho A.V., Hopcroft J.E., Ullman J.D., *The Design and Analysis of Computer Algorithms*, Addison-Wesley, 1982.

Theoretical coverage of the design and analysis of computer algorithms.

Beckman F.S., *Mathematical Foundations of Programming*, Addison-Wesley, 1981

Good clear coverage of the theoretical basis of computing.

Bulloff J.J., Holyoke T.C., Hahn S.W., *Foundations of Mathematics — Symposium Papers Commemorating the 60th Birthday of Kurt Gödel*, Springer-Verlag, 1969.

The comment by John von Neumann highlights the importance of Gödel's work, *.. Kurt Gödel's achievement in modern logic is singular and monumental — indeed it is more than a monument, it is a landmark which will remain visible far in space and time. Whether anything comparable to it has occurred in the logic of modern times may be debated. In any case, the conceivable proxima are very, very few. The subject of logic has certainly changed its nature and possibilities with Gödel's achievement.*

Dahl O.J., Dijkstra E.W., Hoare C.A.R., *Structured Programming*, Academic Press, 1972.

This is the seminal book on structured programming.

Davis M., *Computability and Unsolvability*, Dover, 1982.

The book is an introduction to the theory of computability and noncomputability — the theory of recursive functions in mathematics. Not for the mathematically faint hearted!

Davis W.S., *Systems Analysis and Design*, Addison-Wesley, 1983.

Good introduction to systems analysis and design, with a variety of case studies. Also looks at some of the tools available to the systems analyst.

Fogelin R.J., *Wittgenstein*, Routledge and Kegan Paul, 1980.

The book provides a gentle introduction to the work of the philosopher Wittgenstein, who examined some of the philosophical problems associated with logic and reason.

Gödel K., *On Formally Undecidable Propositions of Principia Mathematica and Related Systems*, Oliver and Boyd, 1962.

An English translation of Gödel's original paper by Meltzer, with quite a lengthy introduction by R.B. Braithwaite, then Knightbridge Professor of Moral Philosophy at Cambridge University, England, and classified under philosophy at the library at King's, rather than mathematics.

Hofstadter D.,*The Eternal Golden Braid*, Harvester Press, 1979.

A very readable coverage of paradox and contradiction in art, music and logic, looking at the work of Escher, Bach and Gödel, respectively.

Hopcroft J.E., Ullman J.D., *Introduction to Automata Theory, Languages and Computation*, Addison-Wesley, 1979.

Comprehensive coverage of the theoretical basis of computing.

Kernighan B.W., Plauger P.J., *Software Tools,* Addison-Wesley, 1976.

Interesting essays on the program development process, originally using a nonstandard variant of Fortran. Also available using Pascal.

Knuth D.E., *The Art of Computer Programming*, Addison-Wesley,

Vol 1. *Fundamental Algorithms*, 1974

Vol 2. *Semi-numerical Algorithms*, 1978

Vol 3. *Sorting and Searching*, 1972

Contains interesting insights into many aspects of algorithm design. Good source of specialist algorithms, and Knuth writes with obvious and infectious enthusiasm (and erudition).

Millington D., *Systems Analysis and Design for Computer Applications*, Ellis Horwood, 1981.

Short and readable introduction to systems analysis and design.

Wirth N., *Program Development by Stepwise Refinement*, Communications of the ACM, April 1971, Volume 14, Number 4, pp. 221-227.

Clear and simple exposition of the ideas of stepwise refinement.

6

Introduction to Programming Languages

"We have to go to another language in order to think clearly about the problem."

Samuel R. Delany, *Babel-17*

Aims

The primary aim of this chapter is to provide a short history of program language development and give some idea as to the concepts that have had an impact on Fortran 95. It concentrates on some but not all of the major milestones of the last 40 years, in roughly chronological order. The secondary aim is to show the breadth of languages available. The chapter concludes with coverage of a small number of more specialised languages.

6 Introduction to Programming Languages

It is important to realise that programming languages are a recent invention. They have been developed over a relatively short period — 45 years — and are still undergoing improvement. Time spent gaining some historical perspective will help you understand and evaluate future changes. This chapter starts right at the beginning and takes you through some, but not all, of the developments during this 45 year span. The bulk of the chapter describes languages that are reasonably widely available commercially, and therefore ones that you are likely to meet. The chapter concludes with a coverage of some more specialised and/or recent developments.

6.1 Some early theoretical work

Some of the most important early theoretical work in computing was that of *Turing* and *von Neumann.* Turing's work provided the base from which it could be shown that it was possible to get a machine to solve problems. The work of von Neumann added the concept of storage and combined with Turing's work to provide the basis for most computers designed to this day.

6.2 What is a programming language?

For a large number of people a programming language provides the means of getting a digital computer to solve a problem. There is a wide range of problems and an equally wide range of programming languages, with particular languages being suited to a particular class of problems, all of which often appears bewildering to the beginner.

6.3 Program language development and engineering

There is much in common between the development of programming languages and the development of anything from the engineering world. Consider the car: old cars offer much of the same functionality as more modern ones, but most people prefer driving newer models. The same is true of programming languages, where you can achieve much with the older languages, but the newer ones are easier to use.

6.4 The early days

A concept that proves very useful when discussing programming languages is that of the level of a machine. By this is meant how close a language is to the underlying machine that the program *runs* on. In the early days of programming (up to 1954) there were only two broad categories: machine languages and assemblers. The language that digital machines use is that of 0 and 1, i.e., they are binary devices. Writing a program in terms of patterns of 0 and 1 was not particularly satisfactory and the capability of using more meaningful mnemonics was soon in-

troduced. Thus it was realised quite quickly that one of the most important aspects of programming languages is that they have to be read and understood by *both* machines and humans.

6.4.1 Fortran — The Early Days

The next stage was the development of higher-level languages. The first of these was *Fortran* and it was developed over a 3 year period from 1954 to 1957 by an IBM team led by John Backus. This group achieved considerable success, and helped to prove that the way forward lay with high-level languages for computer-based problem solving. Fortran stands for *for*mula *tran*slation and was used mainly by people with a scientific background for solving problems that had a significant arithmetic content. It was thus relatively easy, for the time, to express this kind of problem in Fortran.

By 1966 and the first standard Fortran:

- Was widely available.
- Was easy to teach.
- Had demonstrated the benefits of subroutines and independent compilation.
- Was relatively machine independent.
- Often had very efficient implementations.

Possibly the single most important fact about Fortran was, and still is, its widepread usage in the scientific community.

6.4.2 Fortran 77

The next standard in 1977 (actually 1978, and thus out by one — a very common programming error, more of this later!) added character handling, but little else in the way of major new features, really tidying up some of the deficiencies of the 1966 standard.

6.4.3 Cobol

The business world also realised that computers were useful and several languages were developed, including FLOWMATIC, AIMACO, Commercial Translator and FACT, leading eventually to Cobol — *Co*mmon *B*usiness *O*rientated *L*anguage. There is a need in commercial programming to describe data in a much more complex fashion than for scientific programming, and Cobol had far greater capability in this area than Fortran. The language was unique at the time in that a group of competitors worked together with the objective of developing a language that would be useful on machines used by other manufacturers.

The contributions made by Cobol include:

- Firstly the separation among:
  - The task to be undertaken.
  - The description of the data involved.
  - The working environment in which the task is carried out.
- Secondly a data description mechanism that was largely machine independent.
- Thirdly its effectiveness for handling large files.
- Fourthly the benefit to be gained from a programming language that was easy to read.

Modern developments in computing — of report generators, file-handling software, fourth-generation development tools, and especially the increasing availability of commercial relational database management systems — are gradually replacing the use of Cobol, except where high efficiency and/or tight control are required.

6.4.4 Algol

Another important development of the 1950s was Algol. It had a history of development from Algol 58, the original Algol language, through Algol 60 eventually to the Revised Algol 60 Report. Some of the design criteria for Algol 58 were:

- The language should be as close as possible to standard mathematical notation and should be *readable* with little further explanation.
- It should be possible to use it for the description of computing processes in publications.
- The new language should be mechanically translatable into machine programs.

A sad feature of Algol 58 was the lack of any input/output facilities, and this meant that different implementations often had incompatible features in this area.

The next important step for Algol occurred at a UNESCO-sponsored conference in June 1959. There was an open discussion on Algol and the outcome was Algol 60, and eventually the Revised Algol 60 Report.

It was at this conference that John Backus gave his now famous paper on a method for defining the syntax of a language, called Backus Normal Form, or BNF. The full significance of the paper was not immediately recognised. However, BNF was to prove of enormous value in language definition, and helped provide an interface point with computational linguistics.

The contributions of Algol to program language development include:

- Block structure.
- Scope rules for variables because of block structure.
- The BNF definition by Backus — most languages now have a formal definition.
- The support of recursion.
- Its offspring.

Thus Algol was to prove to make a contribution to programming languages that was never reflected in the use of Algol 60 itself, in that it has been the parent of one of the main strands of program language development.

6.5 Chomsky and program language development

Programming languages are of considerable linguistic interest, and the work of Chomsky in 1956 in this area was to prove of inestimable value. Chomsky's system of transformational grammar was developed in order to give a precise mathematical description to certain aspects of language. Simplistically, Chomsky describes grammars, and these grammars in turn can be used to define or generate corresponding kinds of languages. It can be shown that for each type of grammar and language there is a corresponding type of machine. It was quickly realised that there was a link with the earlier work of Turing.

This link helped provide a firm scientific base for programming language development, and modern compiler writing has come a long way from the early work of Backus and his team at IBM. It may seem unimportant when playing a video game at home or in an arcade, but for some it is very comforting that there is a firm theoretical basis behind all that fun.

6.6 Lisp

There were also developments in very specialized areas. List processing was proving to be of great interest in the 1950s and saw the development of IPLV between 1954 and 1958. This in turn led to the development of Lisp at the end of the 1950s. Lisp has proved to be of considerable use for programming in the areas of artificial intelligence, playing chess, automatic theorem proving and general problem solving. It was one of the first languages to be interpreted rather than compiled. Whilst interpreted languages are invariably slower and less efficient in their use of the underlying computer systems than compiled languages, they do provide great opportunities for the user to explore and try out ideas whilst sitting at a terminal. The power that this gives to the computational problem solver is considerable.

Possibly the greatest contribution to program language development made by Lisp was its functional notation. One of the major problems for the Lisp user has been the large number of Lisp flavours, and this has reduced the impact that the language has had and deserved.

6.7 Snobol

Snobol was developed to aid in string processing, which was seen as an important part of many computing tasks, e.g., parsing of a program. Probably the most important thing that Snobol demonstrated was the power of pattern matching in a programming language, e.g., it is possible to define a pattern for a title that would include Mr, Mrs, Miss, Rev, etc., and search for this pattern in a text using Snobol. Like Lisp it is generally available as an interpreter rather than a compiler, but compiled versions do exist, and are often called Spitbol. Pattern-matching capabilities are now to be found in many editors and this makes them very powerful and useful tools. It is in the area of text manipulation that Snobol's greatest contribution to program language development lies.

6.8 Second-generation languages

6.8.1 PL/1 and Algol 68

It is probably true that Fortran, Algol 60 and Cobol are the three main first-generation high-level languages. The 1960s saw the emergence of PL/1 and Algol 68. PL/1 was a synthesis of features of Fortran, Algol 60 and Cobol. It was soon realised that whilst PL/1 had great richness and power of expression this was in some ways offset by the greater difficulties involved in language definition and use.

These latter problems were also true of Algol 68. The report introduced its own syntactic and semantic conventions and thus forced another stage in the learning process on the prospective user. However, it has a small but very committed user population who like the very rich facilities provided by the language.

6.8.2 Simula

Another strand that makes up program language development is provided by Simula, a general purpose programming language developed by Dahl, Myhrhaug and Nygaard of the Norwegian Computing Centre. The most important contribution that Simula makes is the provision of language constructs that aid the programming of complex, highly interactive problems. It is thus heavily used in the areas of simulation and modelling. It was effectively the first language to offer the opportunity of object orientated programming, and we will come back to this very important development in programming languages later in this chapter.

6.8.3 Pascal

The designer of Pascal, Niklaus Wirth, had participated in the early stages of the design of Algol 68 but considered that the generality and complexity of Algol 68 was a move in the wrong direction. Pascal (like Algol 68) had its roots in Algol 60 but aimed at providing expressive power through a small set of straightforward concepts. This set is relatively easy to learn and helps in producing readable and hence more comprehensible programs.

It became the language of first choice within the field of computer science during the 1970s and 1980s, and the comment by Wirth sums up the language very well: *"although Pascal had no support from industry, professional societies, or government agencies, it became widely used. The important reason for this success was that many people capable of recognising its potential actively engaged themselves in its promotion. As crucial as the existence of good implementations is the availability of documentation. The conciseness of the original report made it attractive for many teachers to expand it into valuable textbooks. Innumerable books appeared between 1977 and 1985, effectively promoting Pascal to become the most widespread language used in introductory programming courses. Good course material and implementations are the indispensable prerequisites for such an evolution."*

6.8.4 APL

APL is another interesting language of the early 1960s. It was developed by Iverson early in the decade and was available by the mid to late 1960s. It is an interpretive vector- and matrix-based language with an extensive set of operators for the manipulation of vectors, arrays, etc., of whatever data type. As with Algol 68 it has a small but dedicated user population. A possibly unfair comment about APL programs is that you do not debug them, but rewrite them!

6.8.5 Basic

Basic stands for *B*eginners *A*ll Purpose *S*ymbolic *I*nstruction *C*ode, and was developed by Kemeny and Kurtz at Dartmouth during the 1960s. Its name gives a clue to its audience and it is very easy to learn. It is generally interpreted, though compiled versions do exist. It is probably the most heavily used language on micros and home computers. It has proved to be well suited to the rapid development of small programs. It is much criticised because it lacks features that encourage or force the adoption of sound programming techniques.

6.8.6 C

There is a requirement in computing to be able to access the underlying machine directly or at least efficiently. It is therefore not surprising that computer professionals have developed high-level languages to do this. This may well seem a

contradiction, but it can be done to quite a surprising degree. Some of the earliest published work was that of Martin Richards on the development of BCPL.

This language directly influenced the work of Ken Thompson and can be clearly seen in the programming languages B and C. The UNIX operating system is almost totally written in C and demonstrates very clearly the benefits of the use of high-level languages wherever possible.

With the widespread use of UNIX within the academic world C gained considerable ground during the 1970s and 1980s. UNIX systems also offered much to the professional software developer, and became widely used for large-scale software development and as Ritchie says: "*C is quirky, flawed, and an enormous success. While accidents of history surely helped, it evidently satisfied a need for a system implementation language efficient enough to displace assembly language, yet sufficiently abstract and fluent to describe algorithms and interactions in a wide variety of environments.*"

6.9 Some other strands in language development

There are many strands that make up program language development and some of them are introduced here.

6.9.1 Abstraction, stepwise refinement and modules

Abstraction has proved to be very important in programming. It enables a complex task to be broken down into smaller parts concentrating on *what* we want to happen rather than *how* we want it to happen. This leads almost automatically to the ideas of stepwise refinement and modules, with collections of modules to perform specific tasks or steps.

6.9.2 Structured programming

Structured programming in its narrowest sense concerns itself with the development of programs using a small but sufficient set of statements and, in particular, control statements. It has had a great effect on program language design, and most languages now support the minimal set of control structures.

In a broader sense structured programming subsumes other objectives, including simplicity, comprehensibility, verifiability, modifiability and maintenance of programs.

6.9.3 Standardisation

The purposes of a standard are quite varied and include:

- **Investment in people:** by this we mean that the time spent in learning a standard language pays off in the long term, as what one learns is applica-

ble on any hardware/software platform that has a standard conformant compiler.

- **Portability:** one can take the code one has written for one hardware/software platform and move it to any hardware/software platform that has a standard conformant compiler.
- **Known reference point:** when making comparisons one starts with reference to the standard first, and then between the additional functionality of the various implementations

These are some but not all of the reasons for the use of standards. Their importance is summed up beautifully by Ronald G. Ross in his introduction to the Cannan and Otten book on the SQL standard: "*Anybody who has ever plugged in an electric cord into a wall outlet can readily appreciate the inestimable benefits of workable standards. Indeed, with respect to electrical power, the very fact that we seldom even think about such access (until something goes wrong) is a sure sign of just how fundamentally important a successful standard can be.*"

Appendix A contains notes on what standards apply at this time for the languages covered.

6.10 Ada

Ada represents the culmination of many years of work in program language development. It was a collective effort and the main aim was to produce a language suitable for programming large-scale and real-time systems. Work started in 1974 with the formulation of a series of documents by the American Department of Defence (DoD), which led to the Steelman documents. It is a modern algorithmic language with the usual control structures and facilities for the use of modules, and allows separate compilation with type checking across modules.

Ada is a powerful and well-engineered language. Its widespread use is certain as it has the backing of the DoD. However, it is a large and complex language and consequently requires some effort to learn. It seems unlikely to be widely used except by a small number of computer professionals.

6.11 Modula

Modula was designed by Wirth during the 1970s at ETH, for the programming of embedded real-time systems. It has many of the features of Pascal, and can be taken for Pascal at a glance. The key new features that Modula introduced were those of processes and monitors.

As with Pascal it is relatively easy to learn and this makes it much more attractive than Ada for most people, achieving much of the capability without the complexity.

6.12 Modula 2

Wirth carried on developing his ideas about programming languages and the culmination of this can be seen in Modula 2. In his words: *"In 1977, a research project with the goal to design a computer system (hardware and software) in an integrated approach, was launched at the Institut fur Informatik of ETH Zurich. This system (later to be called Lilith) was to be programmed in a single high level language, which therefore had to satisfy requirements of high level system design as well as those of low level programming of parts that closely interact with the given hardware. Modula 2 emerged from careful design deliberations as a language that includes all aspects of Pascal and extends them with the important module concept and those of multi-programming. Since its syntax was more in line with Modula than Pascal's the chosen name was Modula 2."*

The language's main additions with regard to Pascal are:

- The module concept, and in particular the facility to split a module into a definition part and an implementation part.
- A more systematic syntax which facilitates the learning process. In particular, every structure starting with a keyword also ends with a keyword, i.e., is properly bracketed.
- The concept of process as the key to multiprogramming facilities.
- So-called low-level facilities, which make it possible to breach the rigid type consistency rules and allow one to map data with Modula 2 structure onto a store without inherent structure.
- The procedure type, which allows procedures to be dynamically assigned to variables.

A sad feature of Modula 2 has been the long time taken to arrive at a standard for the language.

6.13 Other language developments

The following is a small selection of language developments that the authors find interesting — they may well not be included in other people's coverage.

6.13.1 Logo

Logo is a language that was developed by Papert and colleagues at the Artificial Intelligence Laboratory at MIT. Papert is a professor of both mathematics and edu-

cation, and has been much influenced by the psychologist Piaget. The language is used to create learning environments in which children can communicate with a computer. The language is primarily used to demonstrate and help children develop fundamental concepts of mathematics. Probably the *turtle* and *turtle geometry* are known by educationists outside of the context of Logo. Turtles have been incorporated into the Smalltalk computer system developed at Xerox Palo Alto Research Centre — Xerox PARC.

6.13.2 Postscript, TeX and LaTeX

The 1980s saw a rapid spread in the use of computers for the production of printed material. The 3 languages are each used quite extensively in this area.

Postscript is a low-level interpretive programming language with good graphics capabilities. Its primary purpose is to enable the easy production of pages containing text, graphical shapes and images. It is rarely seen by most end users of modern desktop publishing systems, but underlies many of these systems. It is supported by an increasing number of laser printers and typesetters.

TeX is a language designed for the production of mathematical texts, and was developed by Donald Knuth. It linearises the production of mathematics using a standard computer keyboard. It is widely used in the scientific community for the production of documents involving mathematical equations.

LaTex is Leslie Lamport's version of TeX, and is regarded by many as more friendly. It is basically a set of macros that hide raw TeX from the end user. The TeX/LaTeX ratio is probably 1 to 9 (or so I'm reliably informed by a TeXie).

6.13.3 Prolog

Prolog was originally developed at Marseille by a group led by Colmerauer in 1972/73. It has since been extended and developed by several people, including Pereira (L.M.), Pereira (F), Warren and Kowalski. Prolog is unusual in that it is a vehicle for *logic* programming. Most of the languages described here are basically algorithmic languages and require a specification of *how* you want something done. Logic programming concentrates on the *what* rather than the *how*. The language appears strange at first, but has been taught by Kowalski and others to 10-year-old children at schools in London.

6.13.4 SQL

SQL stands for Structured Query Language, and was originally developed by people mainly working for IBM in the San Jose Research Laboratory. It is a relational database language, and enables programmers to define, manipulate and control data in a relational database. Simplistically, a relational database is seen by a user as a collection of tables, comprising rows and columns. It has become the most important language in the whole database field.

6.13.5 ICON

ICON is in the same family as Snobol, and is a high-level general purpose programming language that has most of the features necessary for efficient processing of nonnumeric data. Griswold (one of the original design team for Snobol) has learnt much since the design and implementation of Snobol, and the language is a joy to use in most areas of text manipulation.

It is available for most systems via anonymous FTP from a number of sites on the Internet.

6.14 Object orientated programming — OOP

OOP represents a major advance in program language development. The concepts that this introduces include:

- Classes.
- Objects.
- Messages.
- Methods.

These in turn draw on the ideas found in more conventional programming languages and correspond to

- Extensible data types.
- Instances of a class.
- Dynamically bound procedure calls.
- Procedures of a class.

Inheritance is a very powerful high-level concept introduced with OOP. It enables an existing data type with its range of valid operations to form the basis for a new class, with more data types added with corresponding operations, and the new type is compatible with the original.

As was mentioned earlier, the first language to offer functionality in this area was Simula, and thus the ideas originated in the 1960s. The book *Simula Begin* by Birtwistle, Dahl, Myhrhaug and Nygaard is well worth a read as it represents one of the first books to introduce the concepts of OOP.

6.14.1 Oberon and Oberon 2

As Wirth says: *"The programming language Oberon is the result of a concentrated effort to increase the power of Modula-2 and simultaneously to reduce its complexity. Several features were eliminated, and a few were added in order to increase the expressive power and flexibility of the language."*

Oberon and Oberon 2 are thus developments beyond Modula 2. The main new concept added to Oberon was that of type extension. This enables the construction of new data types based on existing types and allows one to take advantage of what has already been done for that existing type.

Language constructs removed included:

- Variant records.
- Opaque types.
- Enumeration types.
- Subrange types.
- Local modules.
- WITH statement.
- Type transfer functions.
- Concurrency.

The short paper by Wirth provides a fuller coverage. It is available at ETH via anonymous FTP.

6.14.2 Smalltalk

Language plus use of a computer system.

Smalltalk has been under development by the Xerox PARC Learning Research Group since the 1970s. In their words: "*Smalltalk is a graphical, interactive programming environment. As suggested by the personal computer vision, Smalltalk is designed so that every component in the system is accessible to the user and can be presented in a meaningful way for observation and manipulation. The user interface issues in Smalltalk revolve around the attempt to create a visual language for each object. The preferred hardware system for Smalltalk includes a high resolution graphical display screen and a pointing device such as a graphics pen or mouse. With these devices the user can select information viewed on the screen and invoke messages in order to interact with the information.*" Thus Smalltalk represents a very different strand in program language development. The ease of use of a system like this has long been appreciated and was first demonstrated commercially in the Macintosh microcomputers.

Wirth has spent some time at Xerox PARC and has been influenced by their work. In his own words "*the most elating sensation was that after sixteen years of working for computers the computer now seemed to work for me*." This influence can be seen in the design of the Lilith machine, the original Modula 2 engine, and in the development of Oberon as both a language and an operating system.

6.14.3 C++

Stroustrup did his Ph.D thesis at the Computing Laboratory, Cambridge University, England, and worked with Simula. He had previously worked with Simula at the University of Aarhus in Denmark. His comments are illuminating: "*but was pleasantly surprised by the way the mechanisms of the Simula language became increasingly helpful as the size of the program increased. The class and co-routine mechanisms of Simula and the comprehensive type checking mechanisms ensured that problems and errors did not (as I - and I guess most people - would have expected) grow linearly with the size of the program. Instead, the total program acted like a collection of very small (and therefore easy to write, comprehend and debug) programs rather than a single large program.*"

He designed C++ to provide Simula's functionality within the framework of C's efficiency, and he succeeded in this goal as C++ is a widely used object oriented programming language. The major disadvantage now concerns the largely incompatible class libraries that exist. It is hoped that the various standards bodies address this problem in the immediate future.

6.14.4 Java

Bill Joy (of Sun fame) had by the late 1980s decided that C++ was too complicated and that an object oriented environment based upon C++ would be of use. At around about the same time James Gosling (mister emacs) was starting to get frustrated with the implementation of an SGML editor in C++. Oak was the outcome of Gosling's frustration.

Sun over the next few years ended up developing Oak for a variety of projects. It wasn't until Sun developed their own web browser, Hotjava, that Java as a language hit the streets. And as the saying goes *the rest is histor*y.

Java is a relatively simple object oriented language. Whilst it has its origins in C++ it has dispensed with most of the dangerous features. It is OO throughout. Everything is a class.

It is interpreted and the intermediate byte code will run on any machine that has a Java virtual machine for it. This is portability at the object code level, unlike portability at the source code level — which is what we expect with most conventional languages. Some of the safe features of the language include:

- Built in garbage collection.
- No pointers — everything is passed by reference.

It is multithreaded, which makes it a delight for many applications. It has an extensive windows toolkit, the so called AWT that was in the original release of the language and Swing that came in later. It achieves much of what Visual Basic 6

offers but within the framework of a far more powerful language. Development environments are becoming widely available to aid in this task.

A major drawback is the rapid development of the language and the large number of different versions, and further compounded by the different virtual machines available.

6.14.5 Visual Basic

Visual Basic (VB) has developed into one of the most widely used development platforms for Windows. Its main strength is the ability to quickly put a visual interface onto an a program. The following are some dates for the various versions that Microsoft have released:-

- VB 1.0 May 1991 for Windows.
- VB 1.0 for MS-DOS September 1992.
- VB 2.0 November 1992.
- VB 3.0 Summer 1993.
- VB 4.0 August 1995.
- VB 5 February 1997.
- VB 6.0 Summer 1998.
- VB .NET 2002.

Two major drawbacks are:

- It only runs under Microsoft Windows
- It is a proprietary programming language and has been changed several times by Microsoft. The .net version is a backwards incompatible upgrade to previous versions.

It is one of the most widely used programming languages on the Windows platforms.

6.14.6 C#

C# is a new language from Microsoft and is a key part of their .net framework. It is a modern, well-engineered language in the same family of programming languages in terms of syntax as C, C++ and Java. If you have a knowledge of one of these languages it will look very familiar.

One of the design goals was to produce a component oriented language, and to build on the work that Microsoft had done with OLE, ActiveX and COM:

- ActiveX is a set of technologies that enables software components to interact with one another in a networked environment, regardless of the language in which they were created. ActiveX was built on the Component Object Model (COM).
- COM is the object model on which ActiveX Controls and OLE are built. COM allows an object to expose its functionality to other components and to host applications. It defines both how the object exposes itself and how this exposure works across processes and networks. COM also defines the object's life cycle.
- OLE is a mechanism that allows users to create and edit documents containing items or objects created by multiple applications. OLE was originally an acronym for Object Linking and Embedding. However, it is now referred to simply as OLE. Parts of OLE not related to linking and embedding are now part of Active technology.

Other design goals included creating a language:

- Where everything is an object — C# also has a mechanism for going between objects and fundamental types (integers, reals, etc.).
- Which would enable the construction of robust and reliable software — it has garbage collection, exception handling and type safety.
- Which would use a C/C++/Java syntax which is already widely known and thus help programmers converting from one of these languages to C#.

Microsoft has submitted C# to the ECMA for formal standardisation and it became an ISO standard in 2003 - ISO/IEC 23270. Visit

- http://en.wikipedia.org/wiki/C_Sharp_programming_language#Standardization

for up-to-date information on the standardisation effort.

6.15 Fortran 90

Almost as soon as the Fortran 77 standard was complete and published, work began on the next version. The language drew on many of the ideas covered in this chapter and these help to make Fortran 90 a very promising language. Some of the new features included:

- New source form, with blanks being significant and names being up to 31 characters.
- Better control structures.
- Control of the precision of numerical computation.

- Array processing.
- Pointers.
- User defined data types and operators.
- Procedures.
- Modules.
- Recursion.
- Dynamic storage allocation.

We will look into all of these in turn.

6.16 Fortran 1995

Fortran was next standardised in 1996 — yet again out by one! Firstly we have a clear up of some of the areas in the standard that had emerged as requiring clarification. Secondly Fortran 95 added the following major concepts:

- The FORALL construct.
- PURE and ELEMENTAL procedures.
- Implicit initialisation of derived-type objects.
- Initial association status for pointers.

The first two help considerably in parallelization of code.

Minor features include amongst others:

- Automatic deallocation of allocatable arrays.
- Intrinsic SIGN function distinguishes between –0 and +0.
- Intrinsic function NULL returns disconnected pointer.
- Intrinsic function CPU_TIME returns the processor time.
- References to some pure functions are allowed in specification statements.
- Nested WHERE constructs.
- Masked ELSEWHERE construct.
- Small changes to the CEILING, FLOOR, MAXLOC and MINLOC intrinsic functions.

Some of these were added to keep Fortran in line with High Performance Fortran (HPF). More details are given later.

Part 2 of the standard (ISO/IEC 1539-2:1994) adds the functional specification for varying length character data type, and this extends the usefulness of Fortran for character applications very considerably.

6.17 ISO technical reports TR15580 and TR15581

There are two additional reports that have been published on Fortran. TR 15580 specifies three modules that provide access to IEEE floating point arithmetic and TR15581 allows the use of the ALLOCATABLE attribute on dummy arguments, function results and structure components.

6.18 Fortran 2003

The language is known as Fortran 2003 even though the language did not make it through the standardisation process until 2004. It is a major revision.

- Derived-type enhancements: parameterised derived types (allows the kind, length, or shape of a derived type's components to be chosen when the derived type is used), mixed component accessibility (allows different components to have different accessibility), public entities of private type, improved structure constructors, and finalisers.
- Object oriented programming support: enhanced data abstraction (allows one type to extend the definition of another type), polymorphism (allows the type of a variable to vary at run time), dynamic type allocation, SELECT TYPE construct (allows a choice of execution flow depending upon the type a polymorphic object currently has), and type-bound procedures.
- The ASSOCIATE construct (allows a complex expression or object to be denoted by a simple symbol).
- Data manipulation enhancements: allocatable components, deferred-type parameters, VOLATILE attribute, explicit type specification in array constructors, INTENT specification of pointer arguments, specified lower bounds of pointer assignment and pointer rank remapping, extended initialisation expressions, MAX and MIN intrinsics for character type, and enhanced complex constants.
- Input/output enhancements: asynchronous transfer operations (allow a program to continue to process data while an input/output transfer occurs), stream access (allows access to a file without reference to any record structure), user specified transfer operations for derived types, user specified control of rounding during format conversions, the FLUSH statement, named constants for preconnected units, regularisation of input/output keywords, and access to input/output error messages.

- Procedure pointers.
- Scoping enhancements: the ability to rename defined operators (supports greater data abstraction) and control of host association into interface bodies.
- Support for IEC 60559 (IEEE 754) exceptions and arithmetic (to the extent a processor's arithmetic supports the IEC standard).
- Interoperability with the C programming language (allows portable access to many libraries and the low-level facilities provided by C and allows the portable use of Fortran libraries by programs written in C).
- Support for international usage: (ISO 10646) and choice of decimal or comma in numeric formatted input/output.
- Enhanced integration with the host operating system: access to command line arguments and environment variables and access to the processor's error messages (improves the ability to handle exceptional conditions).

It is not clear at this time when compilers will be available that fully conform to the Fortran 2003 standard. At the time of writing this book some compilers had started to implement some of the 2003 features. Up-to-date information can be found at

- http://www.kcl.ac.uk/fortran

where we make available a number of Fortran resources including details of compilers, books, code restructers, etc.

6.19 DTR 19767 enhanced module facilities

The module system in Fortran has a number of shortcomings and this DTR addresses some of the issues.

One of the major issues was the so-called recompilation cascade. Changes to one part of a module forced recompilation of all code that used the module. Modula 2 addressed this issue by distinguishing between the definition or interface and implementation. This can now be achieved in Fortran via submodules.

If a module as specified by International Standard ISO/IEC 1539-1:2004 is used to package proprietary software, the source text of the module cannot be published as authoritative documentation of the interface of the module without either exposing trade secrets or requiring the expense of separating the implementation from the interface every time a revision is published.

Using facilities specified in this technical report, one can easily publish the source text of the module as authoritative documentation of its interface, while witholding

publication of the source text of the submodules that contain the implementation details and the trade secrets embodied within them.

6.20 Internet resources

The Internet provides access to a wealth of information regarding the Fortran family of languages.

6.20.1 Standards information

The official home of the standard is

- http://www.nag.co.uk/sc22wg5/

We recommend visiting the site to keep up to date with Fortran developments.

Their official ftp server can be found at

- ftp://ftp.nag.co.uk/sc22wg5/

Copies of all working documents can be found there.

Also have a look at

- ftp://ftp.nag.co.uk/sc22wg5/N1601-N1650/Index.txt

The following is a version of this file as of November 2004.

```
ISO/IEC JTC1/SC22/WG5 N1650

INDEX OF DOCUMENTS 1601-1650

(Documents enclosed in square brackets are not yet
available)

-----  ----------------------------------------
--------

1601 Draft International Standard for Fortran 2003
(Maine)
1602 Draft TR on Enhanced Module Facilities (Snyder)
1603 Response to the PDTR ballot (Reid)
1604 Report from Netherlands (van Waveren)
1605 Abstract for the TR on Enhanced Module Facilities
(Snyder)
1606 Index of meetings (SD7) (Muxworthy)
1607 SC22 Project Information (SD3) (Reid)
```

```
1608 WG5 Business Plan and Convener's Report to SC22
(Reid)
1609 Result of Enhanced Module Facilities DTR ballot
(JTC 1)
1610 Result of Fortran 2003 DIS ballot (JTC 1)

The documents in square brackets are not yet available.
```

6.20.2 Fortran discussion lists

The first to look at is the Fortran 90 list. Details can be found at

- http://www.jiscmail.ac.uk/lists/COMP-FORTRAN-90.html

If you subscribe you will have access to people involved in Fortran standardisation, language implementors for most of the hardware and software platforms, people using Fortran in many very specialised areas, people teaching Fortran, etc.

There is also a comp.lang.fortran list available via USENET news. This provides access to people worldwide with enormous combined expertise in all aspects of Fortran. Invariably someone will have encountered your problem or one very much like it and have one or more solutions.

There are many people on the Internet who will make the time to provide you with very valuable advice. As a point of network etiquette please do not waste bandwidth with questions that are answered in the FAQ. Please also spend some time developing an understanding of your problem and making some attempt to see if the answer lies in the documentation or manuals. In computing services and technical support many user problems are labelled RTFM — read the fabulous manual.

6.20.3 Other sources

The following URLs are very useful:

- Fortran 90 FAQ, maintained by Michel Olagnon
  - http://www.ifremer.fr/ditigo/molagnon/fortran90/engfaq.html
  - http://www.kcl.ac.uk/fortran
- The Fortran Market, maintained by Walt Brainerd
  - http://www.fortran.com/fortran/market.html
- Fortran90/95 Information, maintained by Mike Metcalf
  - http://www.kcl.ac.uk/fortran
- Fortran FAQ, maintained by Keith Bierman, Sun

- http://www.fortran.com/fortran/FAQ/cont.html
- http://www.kcl.ac.uk/fortran

6.21 Summary

It is hoped that you now have some idea about the wide variety of uses that programming languages are put to.

6.22 Bibliography

Fortran 2003 Standard, ISO/IEC DIS 1539-1:2004(E)

DTR 19767: Enhanced Module Facilities: ISO/IEC TR 19767:2004(E)

The ISO home page is

- http://www.iso.org/

The standard was published on 18th November 2004.

The J3 home page is:

- http://j3-fortran.org

The WG5 home page is:

- http://www.nag.co.uk/sc22wg5/

Both have copies of working documents.

Adobe Systems Incorporated, *Postscript Language: Tutorial and Cookbook*, Addison-Wesley, 1985.

Adobe Systems Incorporated, *Postscript Language: Reference Manual,* Addison-Wesley, 1985.

Adobe System Incorporated, *Postscript Language: Program Design,* Addison-Wesley, 1985.

The three books provide a comprehensive coverage of the facilities and capabilities of Postscript.

ACM SIG PLAN, *History of Programming Languages Conference — HOPL-II*, ACM Press, 1993.

One of the best sources of information on programming language developments, from an historical perspective. There is coverage of Ada, Algol 68, C, C++, CLU, Concurrent Pascal, Formac, Forth, Icon, Lisp, Pascal, Prolog, Smalltalk and Simulation Languages by the people involved in the original design and or implementation. Very highly recommended. This is the second in the HOPL series, and the first was edited by Wexelblat. Details are given later.

Adams J.C., Brainerd W.S., Martin J.T., Smith B.T., Wagener J.L., *Fortran 90 Handbook: Complete ANSI/ISO Reference,* McGraw-Hill, 1992.

A complete coverage of the language. As with the Metcalf and Reid book some of the authors were on the X3J3 committee. Originally expensive, but very thorough.

Annals of the History of Computing, *Special Issue: Fortran's 25 Anniversary,* ACM, Article 6,1, 1984.

Very interesting comments, some anecdotal, about the early work on Fortran.

Barnes J., *Programming in Ada 95,* Addison-Wesley, 1996.

One of the best Ada books. He was a member of the original design team

Bergin T.J., Gibson R.G., *History of Programming Languages*, Addison-Wesley, 1996.

This is a formal book publication of the Cenference Prceedings of HOPL II. The earlier work is based on preprints of the papers.

Birtwistle G.M., Dahl O. J., Myhrhaug B., Nygaard K., *SIMULA BEGIN*, Chartwell-Bratt Ltd, 1979.

A number of chapters in the book will be of interest to programmers unfamiliar with some of the ideas involved in a variety of areas including systems and models, simulation, and co-routines. Also has some sound practical advice on problem solving.

Brinch-Hansen P., *The Programming Language Concurrent Pascal,* IEEE Transactions on Software Engineering, June 1975, 199-207.

Looks at the extensions to Pascal necessary to support concurrent processes.

Cannan S., Otten G., *SQL — The Standard Handbook*, McGraw-Hill, 1993.

Very thorough coverage of the SQL standard, ISO 9075:1992(E).

Chivers I.D., Clark M.W., *History and Future of Fortran,* Data Processing, vol. 27 no 1, January/February 1985.

Short article on an early draft of the standard, around version 90.

Chivers Ian, *Essential C# Fast,* Springer, ISBN 1-85233-562-9

A quick introduction to the C# programming language.

Chivers I.D., *A Practical Introduction to Standard Pascal*, Ellis Horwood, 1986.

A short introduction to Pascal.

Date C.J., *A Guide to the SQL Standard*, Addison-Wesley, 1997.

Date has written extensively on the whole database field, and this book looks at the SQL language itself. As with many of Date's works quite easy to read. Appendix F provides a useful SQL bibliography.

Deitel H.M., Deitel P.J., *Java: How to Program*, Prentice-Hall, 1999.

A very good introduction to Java.

Deitel H.M., Deitel P.J., Nieto T.R., *Simply Visual Basic .Net*, Prentice-Hall, 2003.

Good practical introduction to VB .NET.

Eckstein R., Loy M., Wood D., *Java Swing*, O'Reilly, 1998.

Comprehensive coverage of the visual interface features available in Java.

Flanagan D., *Java in a Nutshell*, O'Reilly, 1996.

Just what you would expect from this series. Very useful reference text.

Geissman L.B., *Separate Compilation in Modula 2 and the Structure of the Modula 2 Compiler on the Personal Computer Lilith*, Dissertation 7286, ETH Zurich

Harbison S.P., Steele G.L., *A C Reference Manual*, Prentice-Hall, 2002.

Very good coverage of the various flavours of C, including K&R C, Standard C 1989, Standard C 1995, Standard C 1999 and Standard C++

Jacobi C., *Code Generation and the Lilith Architecture,* Dissertation 7195, ETH Zurich

Fascinating background reading concerning Modula 2 and the Lilith architecture.

Goldberg A., Robson D., *Smalltalk 80: The Language and its Implementation*, Addison-Wesley, 1983.

Written by some of the Xerox PARC people who have been involved with the development of Smalltalk. Provides a good introduction (if that is possible with the written word) of the capabilities of Smalltalk.

Goos G., Hartmanis J. (Eds), *The Programming Language Ada — Reference Manual,* Springer Verlag, 1981.

The definition of the language.

Griswold R.E., Poage J.F., Polonsky I.P., *The Snobol4 Programming Language*, Prentice-Hall, 1971.

The original book on the language. Also provides some short historical material on the language.

Griswold R.E., Griswold M.T., *The Icon Programming Language*, Prentice-Hall, 1983.

The definition of the language with a lot of good examples. Also contains information on how to obtain public domain versions of the language for a variety of machines and operating systems.

Hoare C.A.R., *Hints on Programming Language Design,* SIGACT/SIGPLAN Symposium on Principles of Programming Languages, October 1973.

The first sentence of the introduction sums it up beautifully: *"I would like in this paper to present a philosophy of the design and evaluation of programming languages which I have adopted and developed over a number of years, namely that the primary purpose of a programming language is to help the programmer in the practice of his art.*"

Jenson K., Wirth N., *Pascal: User Manual and Report*, Springer-Verlag, 1975.

The original definition of the Pascal language. Understandably dated when one looks at more recent expositions on programming in Pascal.

Kemeny J.G., Kurtz T.E., *Basic Programming*, Wiley, 1971.

The original book on Basic by its designers.

Kernighan B.W., Ritchie D.M., *The C Programming Language,* Prentice-Hall, 1978

The original work on the C language, and thus essential for serious work with C.

Kowalski R., *Logic Programming in the Fifth Generation*, The Knowledge Engineering Review, The BCS Specialist Group on Expert Systems.

A short paper providing a good background to Prolog and logic programming, with an extensive bibliography.

Knuth D. E., *The TeXbook*, Addison-Wesley, 1986.

Knuth writes with an tremendous enthusiasm and perhaps this is understandable as he did design TeX. Has to be read from cover to cover for a full understanding of the capability of TeX.

Lyons J., *Chomsky*, Fontana/Collins, 1982.

A good introduction to the work of Chomsky, with the added benefit that Chomsky himself read and commented on it for Lyons. Very readable.

Malpas J., *Prolog: A Relational Language and its Applications*, Prentice-Hall, 1987.

A good introduction to Prolog for people with some programming background. Good bibliography. Looks at a variety of versions of Prolog.

Marcus C., *Prolog Programming: Applications for Database Systems, Expert Systems and Natural Language Systems,* Addison-Wesley.

Coverage of the use of Prolog in the above areas. As with the previous book aimed mainly at programmers, and hence not suitable as an introduction to Prolog as only two chapters are devoted to introducing Prolog.

Metcalf M. and Reid J., *Fortran 90 Explained*, Oxford Science Publications, 1992.

A clear compact coverage of the main features of Fortran 8x. Reid was secretary of the X3J3 committee.

Mossenbeck H., *Object-Orientated Programming in Oberon-2,* Springer-Verlag, 1995.

One of the best introductions to OOP. Uses Oberon-2 as the implementation language. Highly recommended.

Papert S., *Mindstorms - Children, Computers and Powerful Ideas*, Harvester Press, 1980.

Very personal vision of the uses of computers by children. It challenges many conventional ideas in this area.

Sammet J., *Programming Languages: History and Fundamentals*, Prentice-Hall, 1969.

Possibly the most comprehensive introduction to the history of program language development — ends unfortunately before the 1980s.

Sethi R., *Programming Languages: Concepts and Constructs*, Addison-Wesley, 1989.

The annotated bibliographic notes at the end of each chapter and the extensive bibliography make it a useful book.

Reiser M., Wirth N., *Programming in Oberon — Steps Beyond Pascal and Modula,* Addison-Wesley, 1992.

Good introduction to Oberon. Revealing history of the developments behind Oberon.

Reiser M., *The Oberon System: User Guide and Programmer's Manual,* Addision-Wesley, 1991.

How to use the Oberon system, rather than the language.

Stroustroup B., *The C++ Programming Language, 3rd Edition*, Addison-Wesley, 1997.

The C++ book. Written by the designer of the language. Massive improvement over the earlier editions.

Young S. J., *An Introduction to Ada, 2nd Edition*, Ellis Horwood, 1984.

A readable introduction to Ada. Greater clarity than the first edition.

Wexelblat, *History of Programming Languages, HOPL I*, ACM Monograph Series, Academic Press, 1978.

Very thorough coverage of the development of programming languages up to June 1978. Sessions on Fortran, Algol, Lisp, Cobol, APT, Jovial, GPSS, Simula, JOSS, Basic, PL/I, Snobol and APL, with speakers involved in the original languages. Very highly recommended.

Wirth N., *An Assessment of the Programming Language Pascal*, IEEE Transactions on Software Engineering, June 1975, 192-198.

Wirth N., *History and Goals of Modula 2*, Byte, August 1984, 145-152.

Straight from the horse's mouth!

Wirth N., *On the Design of Programming Languages*, Proc. IFIP Congress 74, 386-393, North-Holland.

Wirth N., The Programming Language Pascal, *Acta Informatica* 1, 35-63, 1971.

Wirth N., Modula: a language for modular multiprogramming, *Software Practice and Experience*, 7, 3–35, 1977.

Wirth N., *Programming in Modula 2*, Springer-Verlag, 1983.

The original definition of the language. Essential reading for anyone considering programming in Modula 2 on a long term basis.

Wirth N. Type Extensions, *ACM Trans. on Prog. Languages and Systems*, 10, 2 (April 1988), 2004-214

Wirth N. From Modula 2 to Oberon, *Software — Practice and Experience*, 18,7 (July 1988), 661–670

Wirth N., Gutknecht J., *Project Oberon: The Design of an Operating System and Compiler,* Addison-Wesley, 1992.

Fascinating background to the development of Oberon. Highly recommended for anyone involved in large scale program development, not only in the areas of programming languages and operating systems, but more generally.

7

Introduction to Programming

"Though this be madness, yet there is method in't"
Shakespeare

"'Plenty of practice' he went on repeating, all the time that Alice was getting him on his feet again. 'plenty of practice.'"
The White Knight, *Through the Looking Glass and What Alice Found There,* Lewis Carroll

Aims

The aims of the chapter are:

- To introduce the idea that there is a wide class of problems that can be solved with a computer and, further, that there is a relationship between the kind of problem to be solved and the choice of programming language that is used.
- To give some of the reasons for the choice of Fortran.
- To introduce the fundamental components or kinds of statements to be found in a general purpose programming language.
- To introduce the three concepts of name, type and value.
- To illustrate the above with sample programs based on three of the five intrinsic data types:
    - character, integer and real
- To introduce some of the formal syntactical rules of Fortran.

7 Introduction to Programming

We have seen that an algorithm is a sequence of steps that will solve a part or the whole of a problem. A program is the realisation of an algorithm in a programming language, and there are at first sight a surprisingly large number of programming languages. The reason for this is that there is a wide range of problems that are solved using a computer, e.g., the telephone company generating itemised bills or the meteorological centre producing a weather forecast. These two problems make different demands on a programming language, and it is unlikely that the same language would be used to solve both.

The range of problems that you want to solve will therefore strongly influence your choice of programming language. FORTRAN stands for FORmula TRANslation, which gives a hint of the expected range of problems for which it is suitable.

7.1 Language strengths and weaknesses

Some of the reasons for choosing Fortran are:

- It is a modern and expressive language, with much of the power of Ada without the complexity.
- The language is now suitable for a very wide class of both numeric and nonnumeric problems.
- The language is widely available in both the educational and scientific sectors.
- A lot of software already exists, written in either Fortran 77 or its predecessor, Fortran 66, also known as Fortran IV. This code can be recompiled with standard conforming Fortran 90, 95 and 2003 compilers which protects any major investment in existing code. Some 15% of code worldwide is estimated to be in Fortran.

There are a few warts, however. Given that there has to be backwards compatibility with Fortran 77 some of the syntax is clumsy to say the least. However, a considerable range of problems can now be addressed quite cleanly, if one sticks to a subset of the language and adopts a consistent style.

7.2 Elements of a programming language

As with ordinary (so-called *natural*) languages, e.g., English, French, Gaelic, German, etc., programming languages have rules of syntax, grammar and spelling. The application of these rules in a programming language is more strict. A program has to be unambiguous, since it is a *precise* statement of the actions to be taken. Many everyday activities are rather vaguely defined — *Buy some bread on your way*

home — but we are generally sufficiently adaptable to cope with the variations which occur as a result. If, in a program to calculate wages, we had an instruction *Deduct some money* for tax and insurance we could have an awkward problem when the program calculated completely different wages for the same person for the same amount of work every time it was run. One of the implications of the strict syntax of a programming language for the novice is that apparently silly error messages will appear when one first starts writing programs. As with many other *new* subjects you will have to learn some of the jargon to understand these messages.

Programming languages are made up of statements. We will look at the various kinds of statements briefly below.

7.2.1 Data description statements

These are necessary to describe the kinds of data that are to be processed. In the wages program, for example, there is obviously a difference between people's names and the amount of money they earn, i.e., these two things are not the same, and it would not make any sense adding your name to your wages. The technical term for this is data type — a wage would be of a different data type (a number) to a surname (a sequence of characters).

7.2.2 Control structures

A program can be regarded as a sequence of statements to solve a particular problem, and it is common to find that this sequence needs to be varied in practice. Consider again the wages program. It will need to select among a variety of circumstances (say married or single, paid weekly or monthly, etc,), and also to repeat the program for everybody employed. So there is the need in a programming language for statements to vary and/or repeat a sequence of statements.

7.2.3 Data-processing statements

It is necessary in a programming language to be able to process data. The kind of processing required will depend on the kind or type of data. In the wages program, for example, you will need to distinguish between names and wages. Therefore there must be different kinds of statements to manipulate the different types of data, i.e., *wages* and *names*.

7.2.4 Input and output (I/O) statements

For flexibility, programs are generally written so that the data that they work on exist *outside* the program. In the wages example the details for each person employed would exist in a *file* somewhere, and there would be a *record* for each person in this file. This means that the program would not have to be modified each time a person left, was ill, etc., although the individual records might be updated. It is easier to modify data than to modify a program, and it is less likely to

produce unexpected results. To be able to vary the action there must be some mechanism in a programming language for getting the data *into* and *out of* the program. This is done using input and output statements, sometimes shortened to I/O statements.

Let us now consider a simple program which will read in somebody's first name and print it out:

```
PROGRAM ch0701
!
! This program reads in and prints out a name
!
IMPLICIT NONE
CHARACTER*20 :: First_Name
!
   PRINT *,' Type in your first name.'
   PRINT *,' up to 20 characters'
   READ *,First_Name
   PRINT *,First_Name
!
END PROGRAM ch0701
```

There are several very important points to be covered here, and they will be taken in turn:

- Each line is a statement.
- There is a sequence to the statements. The statements will be processed in the order that they are presented, so in this example the sequence is *print, read, print.*
- The first statement names the program. It makes sense to choose a name that conveys something about the purpose of the program.
- The next three lines are *comment* statements. They are identified by a !. Comments are inserted in a program to explain the purpose of the program. They should be regarded as an integral part of all programs. It is essential to get into the habit of inserting comments into your programs straightaway.
- The IMPLICIT NONE statement means that there has to be explicit typing of each and every data item used in the program. It is good programming practice to include this statement in every program that you write, as it will trap many errors, some often very subtle in their effect. Using an analogy with a play, where there is always a list of the persona involved

before the main text of the play we can say that this statement serves the same purpose.

- The CHARACTER*20 statement is a *type* declaration. It was mentioned earlier that there are different kinds of data. There must be some way of telling the programming language that these data are of a certain type, and that therefore certain kinds of operations are allowed and others are banned or just plain stupid! It would not make sense to add a name to a number, e.g., what does Fred + 10 mean? So this statement defines that the *variable* First_Name is to be of type CHARACTER and only character operations are permitted. The concept of a variable is covered in the next section. Character variables of this type can hold up to 20 characters.
- The PRINT statements print out an informative message to the terminal — in this case a guide as to what to type in. The use of informative messages like this throughout your programs is strongly recommended.
- The READ statement is one of the I/O statements. It is an instruction to *read* from the terminal or keyboard; whatever is typed in from the terminal will end up being associated with the variable First_Name. Input/output statements will be explained in greater detail in later sections.
- The PRINT statement is another I/O statement. This statement will print out what is associated with the variable First_Name and, in this case, what you typed in.
- The END PROGRAM statement terminates this program. It can be thought of as being similar to a full stop in natural language, in that it finishes the program in the same way that a period (.) ends a sentence. Note the use of the name given in the PROGRAM statement at the start of the program.
- Note also the use of the asterisk in three different contexts.
- Indentation has been used to make the structure of the program easier to determine. Programs have to be read by human beings and we will look at this in more depth later.
- Lastly, when you do run this program, character input will terminate with the first blank character.

The above program illustrates the use of some of the statements in the Fortran language. Let us consider the action of the READ * statement in more detail — in particular, what is meant by a variable and a value.

7.3 Variables — name, type and value

The idea of a variable is one that you are likely to have met before, probably in a mathematical context. Consider the following:

circumference = 2 π r

This is an equation for the calculation of the circumference of a circle. The following represents a translation of this into Fortran:

circumference = 2 * pi * radius

There are a number of things to note about this equation:

- Each of the *variables* on the right-hand side of the equals sign (pi and radius) will have a *value*, which will allow the evaluation of the expression.
- When the expression is fully evaluated the value is assigned to the variable on the left-hand side of the equals sign.
- In mathemetics the multiplication is implied in Fortran we have to use the * operator to indicate that we want to multiply 2 by pi by the radius.
- We do not have access to mathematical symbols like π in Fortran but have to use variable names based on letters from the Roman alphabet.

The whole line is an example of an *arithmetic assignment statement* in Fortran.

The following arithmetic assignment statement illustrates clearly the concepts of name and value, and the difference in the equals sign in mathematics and computing:

$i = i + 1$

In Fortran this reads as take the current value of the variable i and add one to it, store the new value back into the variable i, i.e., i takes the value i+1. Algebraically,

$i = i + 1$

does not make any sense.

Variables can be of different types. Table 7.1 shows some of those available in Fortran.

Variable_name	Data_type	Value_stored
Temperature	REAL	28.55
Number_of_People	INTEGER	100
First_Name	CHARACTER	Jane

Table 7.1 Variable, Type and Value

Note the use of capitalisation and underscores to make the variable names easier to read.

The concept of data type seems a little strange at first, especially as we commonly think of integers and reals as numbers. However, the benefits to be gained from this distinction are considerable. This will become apparent after you have written several programs.

Let us now consider another program, one that reads in three numbers, adds them up and prints out both the total and the average:

```
PROGRAM ch0702
!
! This program reads in three numbers and sums
! and averages them
!
IMPLICIT NONE
REAL :: N1,N2,N3,Average = 0.0, Total = 0.0
INTEGER :: N = 3
   PRINT *,' Type in three numbers.'
   PRINT *,' Separated by spaces or commas'
   READ *,N1,N2,N3
   Total= N1 + N2 + N3
   Average=Total/N
   PRINT *,'Total of numbers is ',Total
   PRINT *,'Average of the numbers is ',Average
END PROGRAM ch0702
```

7.4 Notes

The program has been given a name that means something.

There are comments at the start of the program describing what it does.

The IMPLICIT NONE statement ensures that all data items introduced have to occur in a type declaration.

The next two statements are type declarations. They define the variables to be of *real* or *integer* type. Remember integers are *whole* numbers, whereas real numbers are those which have a *decimal point.* For example, 2 is an integer and 2.7, 2.00000001, and 2.0 are all real numbers. One of the fundamental distinctions in Fortran is between integers and reals. Type declarations must always come at the start of a program, before any *processing* is done. Note that the variables have been given sensible names to aid in making the program easier to understand.

The variables Average, Total and N are also given initial values within the type declaration. Variables are initially undefined in Fortran, so the variables N1, N2, N3 fall into this category, as they have not been given values at the time that they are declared.

The first PRINT statement makes a text message (in this case what is between the apostrophes) appear at the terminal. As was noted earlier, it is good practice to put out a message like this so that you have some idea of what you are supposed to type in.

The READ statement looks at the input from the keyboard (i.e., what you type) and in this instance associates these values with the three variables. These values can be separated by commas (,), spaces ( ), or even by pressing the carriage return key, i.e., they can appear on separate lines.

The next statement actually does some data processing. It adds up the *values* of the three variables (N1, N2, and N3) and assigns the result to the variable Total. This statement is called an *arithmetic assignment statement*, and is covered more fully in the next chapter.

The next statement is another data-processing statement. It calculates the average of the numbers entered and assigns the result to Average. We could have actually used the value 3 here instead, i.e., written Average=Total/3 and have exactly the same effect. This would also have avoided the type declaration for N. However, the original example follows established programming practice of declaring all variables and establishing their meaning unambiguously. We will see further examples of this type throughout the book.

Indentation has been used to make the structure of the program easier to determine.

The sum and average are printed out with suitable captions or headings. **Do not** write programs without putting captions on the results. It is too easy to make mistakes when you do this, or even to forget what each number means.

Finally we have the end of the program and again we have the use of the name in the PROGRAM statement.

7.5 Some more Fortran rules

There are certain things to learn about Fortran which have little immediate meaning and some which have no logical justification at all, other than historical precedence. Why is a cat called a cat? At the end of several chapters there will be a brief summary of these *rules* or regulations when necessary. Here are a few:

- Source is free format.
- Lowercase letters are permitted, but not required to be recognised.
- Multiple statements may appear on one line and are separated by the semicolon character.
- There is an order to the statements in Fortran. Within the context of what you have covered so far, the order is:
  - PROGRAM statement.
  - Type declarations, e.g., IMPLICIT, INTEGER, REAL or CHARACTER.
  - Processing and I/O statements.
  - END PROGRAM statement.
- Comments may appear anywhere in the program, after PROGRAM and before END; they are introduced with a ! character, and can be in line.
- Names may be up to 31 characters in length and include the underscore character.
- Lines may be up to 132 characters.
- Up to 39 continuation lines are allowed (using the ampersand (&) as the continuation character).
- The syntax of the READ and PRINT statement introduced in these examples is
  - READ *format, input-item-list*.
  - PRINT *format, output-item-list*.

- where *format* is * in the examples and called list directed formatting.
- and *input-item-list* is a list of variable names separated by commas.
- and *output-item-list* is a list of variable names and/or a sequence of characters enclosed in either ' or " , again separated by commas.

- If the IMPLICIT NONE statement is not used, variables that are not explicitly declared will default to REAL if the first letter of the variable name is A-H or O-Z, and to INTEGER if the first letter of the variable name is I-N.

7.6 Fortran character set

The following summarises the Fortran character set:

A-Z	Letters	0-9	Digits
_	Underscore		Blank
=	Equal	+	Plus
-	Minus	*	Asterisk
/	Slash or oblique	\	Backslash
(	Left parenthesis	)	Right parenthesis
[	Left square bracket	]	Right square bracket
{	Left curly bracket	}	Right curly bracket
,	Comma	.	Period or decimal point
:	Colon	;	Semicolon
!	Exclamation mark	“	Quotation mark
%	Percent	&	Ampersand
~	Tilde	@	Commercial at
<	Less than	>	Greater than
?	Question mark	'	Apostrophe
`	Grave accent	^	Circumflex accent
|	Vertical bar or line	$	Currency symbol
#	Number sign		

7.7 Good programming guidelines

The following are guidelines, and do not form part of the Fortran language definition:

- Use comments to clarify the purpose of both sections of the program and the whole program.
- Choose meaningful names in your programs.
- Use indentation to highlight the structure of the program. Remember that the program has to be read and understood by both humans and a computer.
- Use IMPLICIT NONE in all programs you write to minimise errors.

Do not rely on the rules for explicit typing, as this is a major source of errors in programming.

7.8 Compilers

A number of hardware platforms, operating systems and compilers have been used when writing this book and the two earlier books on Fortran 95 and Fortran 90:

- DEC VAX under VMS and later OPEN VMS with the NAG Fortran 90 compiler.
- DEC Alpha under OPEN VMS using the DEC Fortran 90 compiler.
- Sun Ultra Sparc under Solaris:
  - NAGACE F90 compiler.
  - NAGWare F95 compiler.
  - Sun (Release 1.x) F90 compiler.
  - Sun (Release 2.x) F90 compiler.
- PCs under DOS and Windows:
  - DEC/Compaq Fortran 90 and Fortran 95 compilers.
  - Intel Compiler (7.x, 8.x).
  - Lahey Futitsu Fortran 95 (5.7).
  - NAG Fortran 95 Compiler.
  - NAG Salford Fortran 90 Compiler.
  - Salford Fortran 95 Compiler.

- PCs under Linux:
  - Intel Compiler.
  - Lahey Fujitsu Fortran 95 Pro (6.1).
  - NAG Fortran 95 (4.x, 5.x).

It is very illuminating to use more than one compiler whilst developing programs.

7.9 Program development

A number of ways of developing programs have been used, including:

- Using DEC terminals to log into the DEC VAX and DEC Alpha systems.
- Using PCs running terminal emulation software to log into the DEC VAX and DEC Alpha systems.
- Using terminal emulation software to log into the SUN Ultra Sparc.
- Using X-Windows software to log into the SUN Ultra Sparc systems.
- Using a DOS box and simple command line prompt.
- Using an integrated development environment, e.g., Microsoft Developer Studio.

It is likely that you will end up doing at least one of the above and probably more. The key stages involved are:

- Creating and making changes to the Fortran program source.
- Saving the file.
- Compiling the program:
  - If there are errors you must go back to the Fortran source and make the changes indicated by the compiler error messages.
- Linking if successful to generate an executable:
  - Automatic link. This happens behind the scenes and the executable is generated for you immediately.
  - Manual link. You explicitly invoke the linker to generate the executable.
- Running the program.
- Determining whether the program actually works and gives the results expected.

These steps must be taken regardless of the hardware platform, operating system and compiler you use. Some people like working at the operating system prompt (e.g., DOS or UNIX), and others prefer working within a development environment. Both have their strengths and weaknesses.

7.10 Problems

1. Compile and run example 1 in this chapter. Experiment with the following types of input.

Ian

Ian Chivers

"Jane Margaret Sleightholme"

2. Compile and run example 2 in this chapter.

Think about the following points:

- Is there a difference between separating the input by spaces or commas?
- Do you need the decimal point?
- What happens when you type in too many data?
- What happens when you type in too few data?

If you have access to more than one compiler repeat the above and compare the results.

3. Write a program that will read in your name and address and print them out in reverse order.

Think about the following points:

- How many lines are there in your name and address?
- What is the maximum number of characters in the longest line in your name and address?
- What happens at the first blank character of each input line?
- Which characters can be used in Fortran to enclose each line of text typed in and hence not stop at the first blank character?
- If you use one of the two special characters to enclose text what happens if you start on one line and then press the return key before terminating the text?

The action here will vary between Fortran implementations.

8

Arithmetic

"Taking Three as the subject to reason about —
A convenient number to state —
We add Seven, and Ten, and then multiply out
By One Thousand diminished by Eight.
The result we proceed to divide, as you see,
By Nine Hundred and Ninety and Two:
Then subtract Seventeen, and the answer must be
Exactly and perfectly true."

Lewis Carroll, *The Hunting of the Snark*

"Round numbers are always false."

Samuel Johnson

Aims

The aims of this chapter are to introduce:

- The rules for the evaluation of arithmetic expressions to ensure that they are evaluated as you intend.
- The idea of truncation and rounding applied to reals.
- The use of the PARAMETER statement to define or set up constants.
- The concepts and ideas involved in numerical computation, including:
    - Specifying data types using kind-type parameters.
    - The concept of numeric models and positional number systems for integer and real arithmetic and their implementation on binary devices.
    - Testing the numerical representation of different kind types on a system.

8 Arithmetic

Most problems in the academic and scientific communities require arithmetic evaluation as part of the algorithm. As the rules for the evaluation of arithmetic in Fortran may differ from those that you are probably familiar with, you need to learn the Fortran rules thoroughly. In the previous chapter, we introduced the arithmetic assignment statement, emphasising the concepts of name, type and value. Here we will consider the way that arithmetic expressions are evaluated in Fortran.

Table 8.1 lists the five arithmetic operators available in Fortran.

Mathematical operation	Fortran symbol or operator
Addition	+
Subtraction	–
Division	/
Multiplication	*
Exponentiation	**

Table 8.1 Fortran Operators

Exponentiation is raising to a power. Note that the exponentiation operator is the * character *twice*.

The following are some examples of valid arithmetic assignment statements in Fortran:

```
Taxable_Income = Gross_Wage - Personal_allowance
Cost = Bill + Vat + Service
Delta = Deltax/Deltay
Area = Pi * Radius * Radius
Cube = Big ** 3
```

The above expressions are all simple, and there are no problems when it comes to evaluating them. However, now consider the following:

```
Tax = Gross_Wage - Personal_Allowance * Tax_Rate
```

This is a poorly written arithmetic expression. There is a choice of doing the subtraction before or after the multiplication. Our everyday experience says that the subtraction should take place before the multiplication. However, if this expression were evaluated in Fortran the *multiplication* would be done before the subtraction. A complete program to show the correct form in Fortran is as follow:

```
PROGRAM ch0801
IMPLICIT NONE
!
! Example of a Fortran program to calculate net pay
! given an employee's gross pay
!
REAL             :: Gross_wage, Net_wage, Tax
REAL             :: Tax_rate = 0.25
INTEGER          :: Personal_allowance = 4800
CHARACTER*60     :: Their_Name
   PRINT *,'Input employees name'
   READ *,Their_Name
   PRINT *,'Input Gross wage'
   READ *,Gross_wage
   Tax = (Gross_wage - Personal_allowance) * Tax_rate
   Net_wage = Gross_wage - Tax
   PRINT *,'Employee: ',Their_Name
   PRINT *,'Gross Pay: ', Gross_wage
   PRINT *,'Tax: ',Tax
   PRINT *,'Net Pay:',Net_wage
END PROGRAM ch0801
```

We need to look at three areas here:

- The rules for forming expressions — the syntax.
- The rules for interpreting expressions — the semantics.
- The rules for evaluating expressions — optimisation.

The syntax rules determine which expressions are valid. The semantics determine a valid interpretation, and once this has been done the compiler can replace the expression with any other one that is mathematically equivalent, generally in the interests of optimisation.

The rules for the evaluation of expressions in Fortran are as follows:

- Brackets are used to define priority in the evaluation of an expression.

- Operators have a hierarchy of priority — a precedence. The hierarchy of operators is:
  - **Exponentiation:** when the expression has multiple exponentiation, the evaluation is from right to left. For example,

    L = I ** J ** K

    is evaluated by first raising J to the power K, and then using this result as the exponent for I; more explicitly,

    L = I ** (J ** K)

    Although this is similar to the way in which we might expect an algebraic expression to be evaluated, it is not consistent with the rules for multiplication and division, and may lead to some confusion. When in doubt, use brackets.
  - **Multiplication and division:** within successive multiplications and divisions, the rules regarding any mathematically equivalent expression means that you must use brackets to ensure the evaluation you want For example, with

    A = B * C / D * E

    for noninteger numeric types the compiler does not necessarily evaluate in a left to right manner, i.e., evaluate B times C, then divide the result by D and finally take that result and multiply by E.
  - **Addition and subtraction:** as for multiplication and division the rules regarding any equivalent expression apply. However, it is seldom that the order of addition and subtraction is important, unless other operators are involved.

The following are all examples of valid arithmetic expressions in Fortran:

```
Slope = (Y1-Y2)/(X1-X2)
X1 = (-B+((B*B-4*A*C)**0.5))/(2*A)
Q = Mass_D/2*(Mass_A*Veloc_A/Mass_D)**2 + &
      ((Mass_A * Veloc_A)**2)/2
```

Note that brackets have been used to make the order of evaluation more obvious. It is often possible to write involved expressions without brackets, but, for the sake of clarity, it is often best to leave the brackets in, even to the extent of inserting a few extra ones to ensure that the expression is evaluated correctly. The expression will be evaluated just as quickly with the brackets as without. Also note that none

of the expressions is particularly complex. The last one is about as complex as you should try: with more complexity than this it is easy to make a mistake.

The rule regarding any equivalent expression means if A, B and C are numeric then the following are true:

$$A + B = B + A$$

$$-A + B = B - A$$

$$A + B + C = A + (B + C)$$

The last is nominally evaluated left to right, as the additions are of equal precedence:

$$A * B = B * A$$

$$A * B * C = A * (B * C)$$

and again the last is nominally evaluated left to right, as the multiplications are of equal precedence:

$$A * B - A * C = A * (B - C)$$

$$A / B / C = A / (B * C)$$

The last is true for noninteger numeric types only.

Problems arise when the value that a *faulty* expression yields lies within the range of expected values and the error may well go undetected. This may appear strange at first, but a computer does exactly what it is instructed to do. If, through a misunderstanding on the part of a programmer, the program is syntactically correct but logically wrong from the point of view of the problem definition, then this will not be spotted by the compiler. If an expression is complex, break it down into successive statements with elements of the expression on each line, e.g.,

```
Temp = B * B - 4 * A * C
X1 = ( - B + ( Temp ** 0.5 )) / ( 2 * A )
```

and

```
Moment = Mass_A * Veloc_A
Q = Mass_D / 2 * ( Moment / Mass_D ) **2 + &
   ( Moment **2) / 2
```

8.1 Rounding and truncation

When arithmetic calculations are performed one of the following can occur:

- **Truncation.** This operation involves throwing away part of the number, e.g., with 14.6 truncating the number to two figures leaves 14.
- **Rounding**. Consider 14.6 again. This is rounded to 15. Basically, the number is changed to the nearest whole number. It is still a real number. What do you think will happen with 14.5; will this be rounded up or down?

You must be aware of these two operations. They may occasionally cause problems in division and in expressions with more than one data type.

To see some of the problems that can occur consider the examples below:

```
PROGRAM ch0802
IMPLICIT NONE
REAL :: A,B,C
INTEGER :: I
   A = 1.5
   B = 2.0
   C = A / B
   I = A / B
   PRINT *,A,B
   PRINT *,C
   PRINT *,I
END PROGRAM ch0802
```

After executing these statements C has the value 0.75, and I has the value zero! This is an example of type conversion across the = sign. The variables on the right are all real, but the last variable on the left is an integer. The value is therefore made into an integer by truncation. In this example, 0.75 is real, so I becomes zero when truncation takes place.

Consider now an example where we assign into a real variable (so that no truncation due to the assignment will take place), but where part of the expression on the righthand side involves integer division:

```
PROGRAM ch0803
IMPLICIT NONE
INTEGER :: I,J,K
REAL :: Answer
   I = 5
   J = 2
   K = 4
   Answer = I / J * K
   PRINT *,I
```

```
   PRINT *,J
   PRINT *,K
   PRINT *,Answer
END PROGRAM ch0803
```

The value of ANSWER is 8, because the I/J term involves integer division. The expected answer of 10 is not that different from the actual one of 8, and it is cases like this that cause problems for the unwary, i.e., where the calculated result may be close to the actual one. In complicated expressions it would be easy to miss something like this.

To recap, truncation takes place in Fortran:

- Across an = sign, when a real is assigned to an integer.
- In integer division.

It is very important to be careful when attempting *mixed mode arithmetic* — that is, when mixing reals and integers. If a real and an integer are together in a division or multiplication, the result of that operation will be real; when addition or subtraction takes place in a similar situation, the result will also be real. The problem arises when some parts of an expression are calculated using integer arithmetic and other parts with real arithmetic:

```
C = A + B - I / J
```

The integer division is carried out before the addition and subtraction; hence the result of I/J is integer, although all the other parts of the expression will be carried out with real arithmetic.

8.2 Time taken for light to travel from the Sun to Earth

How long does it take for light to reach the Earth from the Sun? Light travels 9.46 10^{12} km in 1 year. We can take a year as being equivalent to 365.25 days. (As all school children know, the astronomical year is 365 days, 5 hours, 48 minutes and 45.9747 seconds — hardly worth the extra effort.) The distance between the Earth and Sun is about 150,000,000 km. There is obviously a bit of imprecision involved in these figures, not least since the Earth moves in an elliptical orbit, not a circular one. One last point to note before presenting the program is that the elapsed time will be given in minutes and seconds. Few people readily grasp fractional parts of a year:

```
PROGRAM ch0804
IMPLICIT NONE
REAL :: Light_Minute, Distance, Elapse
INTEGER :: Minute, Second
```

```
REAL , PARAMETER :: Light_Year=9.46*10**12
! Light_year  : Distance travelled by light
! in one year in km
! Light_minute : Distance travelled by light
! in one minute in km
! Distance : Distance from sun to earth in km
! Elapse : Time taken to travel a
! distance (Distance) in minutes
! Minute : Integer number part of elapse
! Second : Integer number of seconds
! equivalent to fractional part of elapse
!
   Light_minute = Light_Year/(365.25 * 24.0 * 60.0)
   Distance = 150.0 * 10 ** 6
   Elapse = Distance / Light_minute
   Minute = Elapse
   Second = (Elapse - Minute) * 60
   Print *,' Light takes ' , Minute,' Minutes'
   Print *,'             ' , Second,' Seconds'
   Print *,' To reach the earth from the sun'
END PROGRAM ch0804
```

The calculation is straightforward; first we calculate the distance travelled by light in 1 minute, and then use this value to find out how many minutes it takes for light to travel a set distance. Separating the time taken in minutes into whole-number minutes and seconds is accomplished by exploiting the way in which Fortran will truncate a real number to an integer on type conversion. The difference between these two values is the part of a minute which needs to be converted to seconds. Given the inaccuracies already inherent in the exercise, there seems little point in giving decimal parts of a second.

It is worth noting that some structure has been attempted by using comment lines to separate parts of the program into fairly distinct chunks. Note also that the comment lines describe the variables used in the program.

Can you see any problems with this example?

8.3 The PARAMETER statement

This statement is used to provide a way of associating a meaningful name with a *constant* in a program. Consider a program where π was going to be used a lot. It would be silly to have to type in 3.14159265358, etc., every time. There would be a lot to type and it is likely that a mistake could be made typing in the correct

value. It therefore makes sense to set up π once and then refer to it by name. However, if PI was just a variable then it would be possible to do the following:

```
REAL :: li,pi
.
pi=3.14159265358
.
pi=4*alpha/beta
.
```

The pi=4*alpha/beta statement should have been li=4*alpha/beta. What has happened is that, through a typing mistake (p and l are close together on a keyboard), an error has crept into the program. It will not be spotted by the compiler. Fortran provides a way of helping here with the PARAMETER statement, which should be preceded with a type declaration. The following are correct examples of the PARAMETER statement:

```
REAL , PARAMETER :: pi=3.14159265358 , C=2.997925
```

and

```
REAL , PARAMETER :: Charge=1.6021917
```

The advantage of the PARAMETER statement is that you could not then assign another value to pi, C or Charge. If you tried to do this, the compiler would generate an error message.

A PARAMETER statement may contain an arithmetic expression, so that some relatively simple arithmetic may be performed in setting up these constants. The evaluation must be confined to addition, subtraction, multiplication, division and integer exponentiation. The following examples help to demonstrate the possibilities:

```
REAL , PARAMETER  :: parsec = 3.08*10**16 , &
                     pi = 3.14159265358 , &
                     radian = 360./pi
```

8.4 Range, precision and size of numbers

The range on integer numbers and the precision and the size of floating point numbers in computing are directly related to the number of bits allocated to their internal representation. Tables 8.2 and 8.3 summarise this information for the two most common bit sizes in use for integers and reals — 32 bits and 64 bits.

Table 8.2 looks at integer numbers.

N bits		Maximum integer
64	(2**63)–1	9,223,372,036,854,774,807
32	(2**31)–1	2,147,483,647

Table 8.2 Word Size and Integer Numbers

Table 8.3 is a corresponding table for real numbers.

N bits	Precision	Smallest real largest real
64	15–18	~ 0.5E–308
		~ 0.8E+308
32	6–9	~ 0.3E–38
		~ 1.7E38

Table 8.3 Word Size and Real Numbers

Note that access to what the hardware supports is dependent on the operating system and compiler as well.

Precision is not the same as accuracy. In this age of digital timekeeping, it is easy to provide an extremely precise answer to the question *What time is it*? This answer need not be accurate, even though it is reported to tenths (or even hundredths!) of a second. Do not be fooled into believing that an answer reported to ten places of decimals must be accurate to ten places of decimals. The computer can only retain a limited precision. When calculations are performed, this limitation will tend to generate inaccuracies in the result. The estimation of such inaccuracies is the domain of the branch of mathematics known as Numerical Analysis.

To give some idea of the problems, consider an imaginary *decimal* computer which retains two significant digits in its calculations. For example, 1.2, 12.0, 120.0 and 0.12 are all given to two-digit precision. Note therefore that 1234.5 would be represented as 1200.0 in this device. When any arithmetic operation is carried out, the result (including any intermediate calculations) will have two significant digits. Thus:

130 + 12 = 140 (rounding down from 142)

and similarly:

17 / 3 = 5.7 (rounding up from 5.666666...)

and:

16 * 16 = 260

Where there are more involved calculations, the results can become even less attractive. Assume we wish to evaluate

(16 * 16) / 0.14

We would like an answer in the region of 1828.5718, or, to two significant digits, 1800.0. If we evaluate the terms within the brackets first, the answer is 260/0.14, or 1857.1428; 1900.0 on the two-digit machine. Thinking that we could do better, we could rewrite the fraction as

(16 / 0.14) * 16

Which gives a result of 1800.0.

Algebra shows that all these evaluations are equivalent if unlimited precision is available.

Care should also be taken when is one is near the numerical limits of the machine. Consider the following:

```
Z = B * C / D
```

where B, C and D are all 10^{30} and we are using 32-bit floating point numbers where the maximum real is approximately 10^{38}. Here the product B * C generates a number of 10^{60} — beyond the limits of the machine. This is called *overflow* as the number is too large. Note that we could avoid this problem by retyping this as

```
Z = B * (C / D)
```

where the intermediate result would now be $10^{30}/10^{30}$, i.e., 1.

There is an inverse called *underflow* when the number is too small, which is illustrated below:

```
Z = X1 * Y1 * Z1
```

where X1 and Y1 are 10^{-20} and Z1 is 10^{20}. The intermediate result of X1 * Y1 is 10^{-40} — again beyond the limits of the machine. This problem could have been overcome by retyping as

```
Z = X1 * (Y1 * Z1)
```

This is a particular problem for many scientists and engineers with all machines that use 32-bit arithmetic for integer and real calculations. This is because there are a number of physical constants (Plank constant, elementary charge, Bohr magneton etc.,) that will cause arithmetic problems due to their size. This is rarely a problem with machines with hardware support for 64-bit arithmetic.

How we get around this problem and how we move our programs from one platform to another making sure that we are working with the same precision and same range of numbers are covered in detail in the next section.

8.5 Health warning: optional reading, beginners are advised to leave until later

It is very important in scientific programming to know the range and precision of data on the hardware platform on which we are working. The facilities provided in Fortran 95 now allow programmers to specify the range and precision they wish to use and the compiler will choose an appropriate type.

If it is not possible to offer the precision and range requested the compiler returns an error code. To avoid this happening the programmer needs to query the computer first for details of its data representations before trying to run a program which specifies range and precision.

In order to do this we use the KIND intrinsic function, (intrinsic functions are covered in depth in Chapter 14 and Appendix D), e.g.:

```
REAL :: X
PRINT *,'Kind number for X = ',KIND(X)
```

This will print out the *kind* number used by your system to represent default REAL variables. These kind numbers are arbitrary and there is usually no meaning attached to them.

Consider the following program, which demonstrates the use of the KIND function:

```
PROGRAM ch0805
IMPLICIT NONE
```

```
INTEGER :: i
REAL :: r
CHARACTER*1 :: c
LOGICAL :: l
COMPLEX :: cp
   PRINT *,' Integer   ',KIND(i)
   PRINT *,' Real     ',KIND(r)
   PRINT *,' Char     ',KIND(c)
   PRINT *,' Logical  ',KIND(l)
   PRINT *,' Complex  ',KIND(cp)
END PROGRAM ch0805
```

It is worthwhile actually typing this program in and seeing what answers you get for the system you are working on. Output from a PC compiler is given below:

```
[FTN90 Version 1.12 Copyright (c)SALFORD SOFTWARE LTD
1992  &  ]
[                      (c)THE NUMERICAL ALGORITHMS
GROUP 1991,1992]
     NO ERRORS  [FTN90]
Program entered
   Integer  3
   Real      1
   Char      1
   Logical  2
   Complex  1
```

The following is the output from the DEC Fortran 90 compiler under OPEN VMS on an Alpha 2100:

```
Program entered
   Integer  4
   Real     4
   Char     1
   Logical  4
   Complex  4
```

Thus it is up to each compiler implementation to decide what kind numbers are associated with each type and kind variation. Thus the kind value on its own should not be used across platforms to try to achieve portability.

In fact, specifying a kind number actually is not what is intended by the Fortran standard, so two intrinsic functions

```
SELECTED_INT_KIND
```

and

```
SELECTED_REAL_KIND
```

are available instead. They are used to specify the range of numbers for integers and the range and precision of numbers for reals, and the compiler will return the appropriate kind numbers that it has assigned to such representations. These kind numbers can be assigned to parameters called *kind type parameters,* which can be used with REAL and INTEGER type declarations. Let's consider the two main numeric types to see how this works.

8.5.1 Selecting different INTEGER kind types

The Fortran standard specifies that only one **integer** kind needs to be available, but often a machine's architecture or compiler implementation will offer more. Most compiler implementations will offer the following:

- 8-bit or one-byte integers.
- 16-bit or two-byte integers.
- 32-bit or four-byte integers.

and 64-bit or eight byte integers will be available on certain platforms and implementations. The most common reason for choosing 8-bit or 16-bit integers is to reduce the memory requirements of your program and the most common reason for choosing 64-bit integers is to solve specialised problems in mathematics requiring large integer numbers.

To choose an integer kind other than the default, you specify the range of the numbers you require it to lie in, in terms of a power of 10; e.g.,

```
INTEGER, PARAMETER :: First = SELECTED_INT_KIND (2)
INTEGER (First) :: I,J
```

selects an integer kind parameter, First, with representation which includes all integers between -10^2 and 10^2, i.e., numbers in the range –100 to 100. The integer kind parameter can be used in brackets after the integer type statement to specify variables of this integer kind, e.g., I and J.

If there is no integer kind representation for the range specified, the SELECTED_INT_KIND function returns –1. Unfortunately it is not possible to then test for –1 in a type statement, i.e., you will get a compile time error message. We suggest that you run the program in Section 8.5.9 to find the limits of your machine's architecture before trying to specify a kind parameter that it can't support.

8.5.2 Selecting different REAL kind types

The Fortran standard specifies that there must be at least two representations of the real type, the default plus one other. Often there are more, depending on what the underlying hardware can support. When working with real data there are two things to specify — range and precision. The precision is the minimum number of significant digits (all floating point numbers are normalised) to which real numbers are stored, and the range is the power of 10 of the largest number to be represented. So, for example, to specify that a variable R has a kind type that supports 15 significant figures and a range $10^{\pm 307}$ we define a real kind parameter, *Long,* and then use this with the REAL type declaration for R as follows:

```
INTEGER, PARAMETER :: Long=SELECTED_REAL_KIND(15,307)
REAL (Long) :: R
```

The only problem is if the underlying hardware can't support this specification, in which case the function will return –1 if the requested precision is unavailable, – 2 if the range is unavailable, and –3 if both are unavailable. As we mentioned earlier with integer kinds, it is not possible to test for negative values in a type declaration, so before trying to use different kind types, or even just the default types, you need to know what kind types your machine supports and their range and precision.

8.5.3 Specifying kind types for literal integer and real constants

A literal constant is a data object whose value cannot change. An integer constant 1 is of default integer kind and a real constant 10.3 is a default real constant. If in a program you have chosen a real kind type, other than the default, then to be consistent and also to make sure that all real arithmetic is done to the precision specified, you need to declare all real constants to be of this kind type. This is done by giving the literal constant followed by an underscore and a kind number or kind type parameter, e.g.

```
constant_kind
```

For the earlier example with a kind type parameter Long, a real literal constant of this type would be given as

```
-22.36_Long
```

It is not recommended to use the actual kind number because, as we have seen, these are not portable across machines.

The convention we use throughout this book if we require a numeric kind type other than the defaults is to specify a kind type parameter, e.g.,

```
INTEGER, PARAMETER :: Long = SELECTED_REAL_KIND(15,307)
```

and then use it with REAL type declarations, e.g.,

```
REAL (Long) :: R
```

This still doesn't make programs completely portable across different hardware platforms, so you will firstly need to run a program which tests the range of data representations. Before doing this we need to know a bit more about the underlying representation of numerical data on computer systems.

8.5.4 Positional number systems

Most people take arithmetic completely for granted and rarely think much about the subject. It is necessary to look at it in a bit more depth if we are to understand what the computer is doing in this area.

Our way of working with numbers is essentially a positional one. When we look at the number 1024, for example, we rarely think of it in terms of 1 * 1000 + 0 * 100 + 2 * 10 + 4 * 1. Thus the normal decimal system we use in everyday life is a positional one, with a base of 10.

We are probably aware that we can use other number bases, and 2, 8 and 16 are fairly common alternate number bases. As the computer is a binary device it uses base 2.

We are also reasonably familiar with a mantissa exponent or floating point combination when the numbers get very large or very small, e.g., a parsec is commonly expressed as 3.08 * 10 ** 16, and here the mantissa is 3.08, and the exponent is 10 ** 16.

The above information will help in understanding the way in which integers and reals are represented on computer systems.

8.5.5 Bit data type and representation model

The model is only defined for positive integers (or cardinal numbers), where they are represented as a sequence of binary digits, and is based on the model:

$$i = \sum_{k=0}^{n-1} b_k \, 2^k$$

where i is the integer value, n is the number of bits, and b_k is a bit value of 0 or 1, with bit numbering starting at 0, and reading right to left. Thus the integer 43 and bit pattern 101011 is given by:

43 = (1 * 32) + (0 * 16) + (1 * 8) + (0 * 4) + (1 * 2) + (1 * 1)

or

$43 = (1 * 2^5) + (0 * 2^4) + (1 * 2^3) + (0 * 2^2) + (1 * 2^1) + (1 * 2^0)$

8.5.6 Integer data type and representation model

The integer data type is based on the model

$$i = s \sum_{k=1}^{q} l_k \, r^{k-1}$$

where i is the integer value, s is the sign, q is the number of digits (always positive), r is the radix or base (integer greater than 1), and l_k is a positive integer (less than r).

A base of 2 is typical so 1023 is

$$1023 = (1 * 2^9) + (1 * 2^8) + (1 * 2^7) + (1 * 2^6) + (1 * 2^5) + (1 * 2^4) + (1 * 2^3) + (1 * 2^2) + (1 * 2^1) + (1 * 2^0)$$

8.5.7 Real data type and representation model

The real data type is based on the model

$$x = s \, b^e \sum_{k=1}^{m} f_k \, b^{-k}$$

where x is the real number, s is the sign, b is the radix or base (greater than 1), m is the number of bits in the mantissa, e is an integer in the range e_{min} to e_{max}, and f_k is a positive number less than b.

This means that with, for example, a 32-bit real there would be 8 bits allocated to the exponent and 24 to the mantissa. One of the bits in each part would be used to represent the sign and is called the sign bit. This reduces the number of bits that can actually be used to represent the mantissa and exponent to 31 and 7, respectively. There is also the concept of normalisation, where the exponent is adjusted so that the most significant bit is in position 22 — bits are typically numbered 0–22, rather than 1–23. This form of representation is not new, and is first documented around 1750 BC, when Babylonian mathematicians used a sexagesimal (radix 60) positional notation. It is interesting that the form they used omitted the exponent!

This is the theoretical basis of the representation of these three data types in Fortran. Remember from Chapter 2 that the computer is essentially a binary device, and works at the lowest level with sequences of zeros and ones.

This information together with the following provide a good basis for writing portable code across a range of hardware.

8.5.8 IEEE 754

The first standard IEEE 754: 1985 covered binary floating point arithmetic. The later IEEE 754: 1987 standard added decimal arithmetic.

A considerable amount of hardware now offers support for the IEEE 754 standard. The standard can be purchased from

- http://standards.ieee.org

Work is under way on the next version and you can find out details of the current state of play at

- http://grouper.ieee.org/groups/754/

There are quite a lot of good links from this site.

8.5.9 Testing the numerical representation of different kind types on a system

You are now ready to write or adapt a program to run on your system in order to test the range of integer kind types and the range and precision of real kind types.

The following program selects several integer and real kind types and by calling the intrinsic functions KIND, HUGE, PRECISION and EPSILON produces most of the information you need to know about for these kind types. Table 8.4 provides details of what these functions do.

Function name	Simple explanation
KIND(X)	Returns the kind type
HUGE(X)	Returns the largest number
PRECISION(X)	Returns the decimal precision
EPSILON(X)	Smallest difference between two reals

Table 8.4 Numeric Query Functions

A complete program using the above is as follows:

```
PROGRAM ch0806
!
! Examples of the use of the kind
```

```
! function and the numeric inquiry functions
!
! Integer arithmetic
!
! 32 bits is a common word size,
! and this leads quite cleanly
! to the following
! 8 bit integers
! -128 to 127 10**2
! 16 bit integers
! -32768 to 32767 10**4
! 32 bit integers
! -2147483648 to 2147483647 10**9
!
! 64 bit integers are increasingly available.
! This leads to
! -9223372036854775808 to
!  9223372036854775807 10**19
!
! You may need to comment out some of the following
! depending on the hardware platform and compiler
! that you use.

INTEGER                          :: I
INTEGER ( SELECTED_INT_KIND( 2)) :: I1
INTEGER ( SELECTED_INT_KIND( 4)) :: I2
INTEGER ( SELECTED_INT_KIND( 9)) :: I3
INTEGER ( SELECTED_INT_KIND(10)) :: I4


! Real arithmetic
!
! 32 and 64 bit reals are normally available.
!
! 32 bit reals 8 bit exponent, 24 bit mantissa
!
! 64 bit reals 11 bit exponent 53 bit mantissa
!
REAL :: R
REAL ( SELECTED_REAL_KIND( 6, 37)) :: R1
REAL ( SELECTED_REAL_KIND(15,307)) :: R2
REAL ( SELECTED_REAL_KIND(15,310)) :: R3
```

```
  PRINT *,' '
  PRINT *,' Integer values'
  PRINT *,' Kind     Huge'
  PRINT *,' '
  PRINT *,' ',KIND(I   ),' ',HUGE(I   )
  PRINT *,' '
  PRINT *,' ',KIND(I1 ),' ',HUGE(I1 )
  PRINT *,' ',KIND(I2 ),' ',HUGE(I2 )
  PRINT *,' ',KIND(I3 ),' ',HUGE(I3 )
  PRINT *,' ',KIND(I4 ),' ',HUGE(I4 )

  PRINT *,' '
  PRINT *,' Real values'
  PRINT *,' Kind     Huge                 ',&
 'Precision        epsilon'
  PRINT *,' '
  PRINT *,' ',KIND(R   ),' ',HUGE(R   ),&
  '             ',PRECISION(R),' ',EPSILON(R)
  PRINT *,' '
  PRINT *,' ',KIND(R1 ),' ',HUGE(R1 ),&
  '             ',PRECISION(R1),' ',EPSILON(R1)
  PRINT *,' ',KIND(R2 ),' ',HUGE(R2 ),&
  ' ',PRECISION(R2),' ',EPSILON(R2)
  PRINT *,' ',KIND(R3 ),' ',HUGE(R3 ),&
  ' ',PRECISION(R3),' ',EPSILON(R3)
END PROGRAM ch0806
```

The output from the Intel compiler under Windows is:

```
  Integer values
  Kind     Huge

               4     2147483647

               1     127
               2     32767
               4     2147483647
               8      9223372036854775807

  Real values
  Kind     Huge                 Precision        epsilon
```

```
                4     3.4028235E+38
6     1.1920929E-07

                4     3.4028235E+38
6     1.1920929E-07
                8     1.797693134862316E+308
15     2.220446049250313E-016
               16
1.189731495357231765085759326628007E+4932
33
  1.925929944387235853055977942584927E-0034
```

The output from the Lahey Fujitsu compiler under Windows is:

```
 Integer values
 Kind     Huge

  4    2147483647

  1    127
  2    32767
  4    2147483647
  8    9223372036854775807

 Real values
 Kind     Huge                  Precision         epsilon

  4    3.40282347E+38                6    1.19209290E-07

  4    3.40282347E+38                6    1.19209290E-07
  8    1.797693134862316E+308    15
2.220446049250313E-16
  16    1.189731495357231765085759326628007E+4932    33
1.925929944387235853055977942584927E-0034
```

The output from the Salford compiler under Windows is:

```
  Integer values
  Kind     Huge
```

```
                3    2147483647

                1            127
                2          32767
                3    2147483647
                4    9223372036854775807

  Real values
  Kind     Huge                  Precision         epsilon

                1      3.402823E+38
6      1.192093E-07

                1      3.402823E+38
6      1.192093E-07
                2          1.797693134862E+0308
15          2.220446049250E-16
                3    1.18973149535723177E+4932
18    1.08420217248550444E-19
```

Run this program on whatever system you have access to and compare the output with the above examples.

8.5.10 Binary representation of different integer kind type numbers

For those who wish to look at the internal binary representation of integer numbers with a variety of kinds, we have included the following program

SELECTED_INT_KIND(2) means provide at least an integer representation with numbers between -10^2 and $+10^2$.

SELECTED_INT_KIND(4) means provide at least an integer representation with numbers between -10^4 and $+10^4$.

SELECTED_INT_KIND(9) means provide at least an integer representation with numbers between -10^9 and $+10^9$.

We use the INT function to convert from one integer representation to another.

We use the logical function BTEST to determine whether the binary value at that position within the number is a zero or a one, i.e., if the bit is set.

I_in_Bits is a character string that holds a direct mapping from the internal binary form of the integer and a text string that prints as a sequence of zeros or ones:

```
PROGRAM ch0807
!
! Use the bit functions in Fortran to write out a
! 32 bit integer number as a sequence of
! zeros and ones
!
INTEGER :: J
INTEGER :: I
INTEGER ( SELECTED_INT_KIND( 2)) :: I1
INTEGER ( SELECTED_INT_KIND( 4)) :: I2
INTEGER ( SELECTED_INT_KIND( 9)) :: I3
CHARACTER (LEN=32) :: I_in_Bits
   PRINT *,' Type in an integer '
   READ * , I
   I1=INT(I,KIND(2))
   I2=INT(I,KIND(4))
   I3=INT(I,KIND(9))
   I_in_Bits=' '
   DO J=0,7
      IF (BTEST(I1,J)) THEN
         I_in_Bits(8-J:8-J)='1'
      ELSE
         I_in_Bits(8-J:8-J)='0'
      END IF
   END DO
   PRINT *,'         1         2         3'
   PRINT *,'12345678901234567890123456789012345678901234567890'
   PRINT *,I1
   PRINT *,I_in_Bits
   DO J=0,15
      IF (BTEST(I2,J)) THEN
         I_in_Bits(16-J:16-J)='1'
      ELSE
         I_in_Bits(16-J:16-J)='0'
      END IF
   END DO
   PRINT *,I2
   PRINT *,I_in_Bits
   DO J=0,31
      IF (BTEST(I3,J)) THEN
         I_in_Bits(32-J:32-J)='1'
      ELSE
```

```
        I_in_Bits(32-J:32-J)='0'
      END IF
   END DO
   PRINT *,I3
   PRINT *,I_in_Bits
END PROGRAM ch0807
```

The DO loop indices follow the convention of an 8-bit quantity starting at bit 0 and ending at bit 7, 16-bit quantities starting at 0 and ending at 15, etc.

The numbers written out follow the conventional mathematical notation of having the least significant quantity at the right-hand end of the digit sequence, i.e., with 127 in decimal we have 1 * 100, 2 * 10 and 7 * 1, so 00100001 in binary means 1 * 32 + 1 * 1 decimal.

Try running this program on the system you are using. Does it produce the results you expect? Experiment with a variety of numbers. Try at least the following 0, +1, –1, –128, 127, 128, –32768, 32767, 32768.

8.5.11 Binary representation of a real number

The following program is a simple variant of the previous one, but we now look at a floating point number:

```
PROGRAM ch0808
!
! Use the bit functions in Fortran to write out a
! 32 bit integer number  equivalenced to a real
! using the transfer intrinsic as a sequence of
! zeros and ones
!
IMPLICIT NONE
INTEGER                                 :: I,J
CHARACTER (LEN=32)                      :: I_in_Bits=" "
REAL                                    :: x=-1.0
   PRINT *,'           1           2           3'
   PRINT *,'12345678901234567890123456789012345678901234567890'
   PRINT *,I_in_Bits
   I=TRANSFER(x,I)
   DO J=0,31
      IF (BTEST(i,J)) THEN
         I_in_Bits(32-J:32-J)='1'
      ELSE
         I_in_Bits(32-J:32-J)='0'
      END IF
```

```
   END DO
   PRINT *,x
   PRINT *,I_in_Bits
END PROGRAM  ch0808
```

We use the intrinsic function transfer to help out here. The BTEST intrinsic takes an integer argument, so we need to copy the bit pattern of the real number into an integer variable.

8.5.12 Summary of how to select the appropriate kind type

To write programs that will perform arithmetically in a similar fashion on a variety of hardware requires an understanding of:

- The integer data representation model and in practice the word size of the various integer kind types.
- The real data representation model and in practice the word size of the various real kind types and the number of bits in both the mantissa and exponent.

Armed with this information we can then choose a kind type that will ensure minimal problems when moving from one platform to another. End of health warning!

8.6 Variable status

Fortran has two concepts regarding the status of a variable: defined and undefined. If a program does not provide an initial value (in a type statement) for a variable then its status is said to be undefined. Consider the following code segment taken from the earlier example that calculated the sum and average of three numbers:

```
REAL :: N1, N2, N3, Average=0.0, Total=0.0
INTEGER :: N=3
```

In the above the variables Average, Total and N all have a defined status. However, N1, N2 and N3 are said to be undefined. The use of undefined values is implementation dependent and therefore not portable. Care must be taken when writing programs to ensure that your variables have a defined status wherever possible. We will look at this area again in subsequent chapters.

8.7 Summary

The following are some practical rules and guidelines:

- Learn the rules for the evaluation of arithmetic expressions.

- Break expressions down where necessary to ensure that the expressions are evaluated in the way you want.
- Take care with truncation owing to integer division in an expression. Note that this will only be a problem where both parts of the division are INTEGER.
- Take care with truncation owing to the assignment statement when there is an integer on the left-hand side of the statement, i.e., assigning a real into an integer variable.
- When you want to set up constants which will remain unchanged throughout the program, use the PARAMETER statement.
- Do not confuse precision and accuracy.
- Learn what the default KINDs are for the numeric types you work with, what the maximum and minimum values and precision are for REAL data, and what the maximum and minimum are for INTEGER data.
- You have been introduced to the use of the functions DIGITS, HUGE and PRECISION, and some of the concepts involved in their use. We will look at functions in much greater depth later on.

8.8 Problems

1. Compile and run examples 1 through 3 in this chapter.

2. Have another look at example 4. Compile and run it. It will generate an error on some systems. Can you see where the error is? Appendix D contains sample output from several compilers.

2.. Write a program to calculate the period of a pendulum. This is given mathematically as

$$t = 2\pi\sqrt{\frac{length}{9.81}}$$

Use the following Fortran arithmetic assignment statement:

```
T = 2 * PI * (LENGTH / 9.81) ** .5
```

The length (LENGTH) is in metres, and the time (T) in seconds. π was given a value earlier in this chapter.

Repeat the above using two other methods. Try a hand-held calculator and a spreadsheet. Do you get the same answers?

3. Base conversion.

In this chapter you have seen a brief coverage of base conversion. The following program illustrates some of the problems that can occur when going from base 10 to base 2 and back again. Which numbers will convert without loss?

```
program base_conversion
real :: x1=1.0
real :: x2=0.1
real :: x3=0.01
real :: x4=0.001
real :: x5=0.0001
  print *,' ',x1
  print *,' ',x2
  print *,' ',x3
  print *,' ',x4
  print *,' ',x5
end program base_conversion
```

Which do you think will provide the same number as originally entered?

4. Simple subtraction. In this chapter we looked at representing floating point numbers in a finite number of bits.

Try the following program:

```
program subtract
real :: a=1.0002
real :: b=1.0001
real :: c
  c=a-b
  print *,a
  print *,b
  print *,c
end program subtract
```

5. Expression equivalence. We introduced some of the rules that apply in Fortran for expression evaluation. In mathematics the following is true:

$(x^2\text{-}y^2) = (x*x\text{-}y*y) = (x\text{-}y)*(x+y)$

Try the following program:

```
program expression_equivalence
!
! simple evaluation of x*x-y*y
! when x and y are similar
```

```
!
! we will evaluate in three ways.
!
real :: x=1.002
real :: y=1.001
real :: t1,t2,t3,t4,t5
   t1=x-y
   t2=x+y
   print *,t1
   print *,t2
   t3=t1*t2
   t4=x**2-y**2
   t5=x*x-y*y
   print *,t3
   print *,t4
   print *,t5
end program expression_equivalence
```

Solve the problem with pencil and paper, calculator and Excel.

The last three examples show that you must be careful when using a computer to solve problems.

6. The following is a simple variant of ch0804. In this case we initialise light year in an assignment statement. Do you think you will get the same results as from running the earlier example? Appendix E contains the output from several compilers.

```
PROGRAM ch0804p
IMPLICIT NONE
REAL :: Light_Minute, Distance, Elapse
INTEGER :: Minute, Second
REAL :: Light_Year
! Light_year  : Distance travelled by light
! in one year in km
! Light_minute : Distance travelled by light
! in one minute in km
! Distance : Distance from sun to earth in km
! Elapse : Time taken to travel a
! distance (Distance) in minutes
! Minute : Integer number part of elapse
! Second : Integer number of seconds
! equivalent to fractional part of elapse
!
```

```
   Light_Year=9.46*10**12
   Light_minute = Light_Year/(365.25 * 24.0 * 60.0)
   Distance = 150.0 * 10 ** 6
   Elapse = Distance / Light_minute
   Minute = Elapse
   Second = (Elapse - Minute) * 60
   Print *,' Light takes ' , Minute,' Minutes'
   Print *,'             ' , Second,' Seconds'
   Print *,' To reach the earth from sun'
END PROGRAM ch0804p
```

8.9 Bibliography

Some understanding of numerical analysis is essential for successful use of Fortran when programming. As Froberg says "*numerical analysis is a science — computation is an art.*" The following are some of the more accessible books available.

Froberg C.E., *Introduction to Numerical Analysis*, Addison-Wesley, 1969.

The short chapter on numerical computation is well worth a read; it covers some of the problems of conversion between number bases and some of the errors that are introduced when we compute numerically. The Samuel Johnson quote owes its inclusion to Froberg!

IEEE, *IEEE Standard for Binary Floating-Point Arithmetic, ANSI/IEEE Std 754-1985*, Institute of Electrical and Electronic Engineers Inc.

The formal definition of IEEE 754.

Knuth D., *Seminumerical Algorithms*, Addison-Wesley, 1969.

A more thorough and mathematical coverage than Wakerly. The chapter on positional number systems provides a very comprehensive historical coverage of the subject. As Knuth points out the floating point representation for numbers is very old, and is first documented around 1750 B.C. by Babylonian mathematicians. Very interesting and worthwhile reading.

Sun, *Numerical Computation Guide*, SunPro, 1993.

Very good coverage of the numeric formats for IEEE Standard 754 for Binary Floating-Point Arithmetic. All SunPro compiler products support the features of the IEEE 754 standard.

Wakerly J.F., *Microcomputer Architecture and Programming*, Wiley, 1981.

The chapter on number systems and arithmetic is surprisingly easy. There is a coverage of positional number systems, octal and hexadecimal number system conversions, addition and subtraction of nondecimal numbers, representation of negative numbers, two's complement addition and subtraction, one's complement addition and subtraction, binary multiplication, binary division, bcd or

binary coded decimal representation and fixed and floating point representations. There is also coverage of a number of specific hardware platforms, including DEC PDP-11, Motorola 68000, Zilog Z8000, TI 9900, Motorola 6809 and Intel 8086. A little old but quite interesting nevertheless.

9

Arrays 1
Some Fundamentals

"Thy gifts, thy tables, are within my brain
Full charactered with lasting memory."

William Shakespeare, *The Sonnets*

"Here, take this book, and peruse it well:
The iterating of these lines brings gold."

Christopher Marlowe, *The Tragical History of Doctor Faustus*

Aims

The aims of the chapter are to introduce the fundamental concepts of arrays and DO loops, in particular:

- To introduce the idea of tables of data and some of the formal terms used to describe them:
  - Array.
  - Vector.
  - List and linear list.
- To discuss the array as a random access structure where any element can be accessed as readily as any other and to note that the data in an array are all of the same type.
- To introduce the twin concepts of data structure and corresponding control structure.
- To introduce the statements necessary in Fortran to support and manipulate these data structures.

9 Arrays 1: Some Fundamentals

9.1 Tables of data

Consider the examples below.

9.1.1 Telephone directory

A telephone directory consists of the following kinds of entries:

Name	Address	Number
Adcroft A.	61 Connaught Road, Roath, Cardiff	223309
Beale K.	14 Airedale Road, Balham	745 9870
Blunt R.U.	81 Stanlake Road, Shepherds Bush	674 4546
...		
...		
...		
Sims Tony	99 Andover Road,Twickenham	898 7330

This *structure* can be considered in a variety of ways, but perhaps the most common is to regard it as a *table* of data, where there are three columns and as many rows as there are entries in the telephone directory.

Consider now the way we extract information from this table. We would scan the name column looking for the name we are interested in, and then read along the row looking for either the address or telephone number, i.e., we are using the name to *look up* the item of interest.

9.1.2 Book catalogue

A catalogue could contain:

Author(s)	Title	Publisher
Carroll L.	Alice through the Looking Glass	Penguin
Steinbeck J.	Sweet Thursday	Penguin
Wirth N.	Algorithms plus Data Structures = Program	Prentice-Hall

Again, this can be regarded as a *table* of data, having three columns and many rows. We would follow the same procedure as with the telephone directory to extract the information. We would use the *Name* to *look up* what books are available.

9.1.3 Examination marks or results

This could consist of:

Name	Physics	Maths	Biology	History	English	French
Fowler L.	50	47	28	89	30	46
Barron L.W	37	67	34	65	68	98
Warren J.	25	45	26	48	10	36
Mallory D.	89	56	33	45	30	65
Codd S.	68	78	38	76	98	65

This can again be regarded as a *table* of data. This example has seven columns and five rows. We would again *look up* information by using the Name.

9.1.4 Monthly rainfall

The following data are the monthly average rainfall for London:

Month	Rainfall
January	3.1
February	2.0
March	2.4
April	2.1
May	2.2
June	2.2
July	1.8
August	2.2
September	2.7
October	2.9
November	3.1
December	3.1

In this table there are two columns and twelve rows. To find out what the rainfall was in July, we scan the table for July in the Month column and locate the value in the same row, i.e., the rainfall figure for July.

These are just some of the many examples of problems where the data that are being considered have a tabular structure. Most general purpose languages therefore have mechanisms for dealing with this kind of structure. Some of the special names given to these structures include:

- Linear list.
- List.
- Vector.
- Array.

The term used most often here, and in the majority of books on Fortran programming, is *array*.

9.2 Arrays in Fortran

There are three key things to consider here:

- The ability to refer to a set or group of items by a single name.
- The ability to refer to individual items or members of this set, i.e., look them up.
- The choice of a control structure that allows easy manipulation of this set or array.

9.3 The DIMENSION attribute

The DIMENSION attribute defines a variable to be an array. This satisfies the first requirement of being able to refer to a set of items by a single name. Some examples are given below:

```
REAL , DIMENSION(1:100) :: Wages
INTEGER , DIMENSION(1:10000) ::  Sample
```

For the variable Wages it is of type REAL and an array of dimension or size 100, i.e., the variable array Wages can hold up to 100 real items.

For the variable Sample it is of type INTEGER and an array of dimension or size 10,000, i.e., the variable Sample can hold up to 10,000 integer items.

9.4 An index

An index enables you to refer to or select individual elements of the array. In the telephone directory, book catalogue, exam marks table and monthly rainfall examples we used the name to index or look up the items of interest. We will give concrete Fortran code for this in the example of monthly rain fall.

9.5 Control structure

The statement that is generally used to manipulate the elements of an array is the DO statement. It is typical to have several statements controlled by the DO statement, and the block of repeated statements is often called a *DO loop*. Let us look at two complete programs that highlight the above.

9.6 Monthly rainfall

Let us look at this earlier example in more depth now. Consider the following:

Month	Associated integer representation	Array and index	Rainfall value
January	1	RainFall(1)	3.1
February	2	RainFall(2)	2.0
March	3	RainFall(3)	2.4
April	4	RainFall(4)	2.1
May	5	RainFall(5)	2.2
June	6	RainFall(6)	2.2
July	7	RainFall(7)	1.8
August	8	RainFall(8)	2.2
September	9	RainFall(9)	2.7
October	10	RainFall(10)	2.9
November	11	RainFall(11)	3.1
December	12	RainFall(12)	3.1

Most of you should be familiar with the idea of the use of an integer as an alternate way of representing a month, e.g., in a date expressed as 1/3/2000, for 1st March 2000 (anglicised style) or January 3rd (americanised style). Fortran, in common with other programming languages, only allows the use of integers as an index into an array. Thus when we write a program to use arrays we have to map between whatever construct we use in everyday life as our index (names in our examples of telephone directory, book catalogue, and exam marks) to an integer

representation in Fortran. The following is an example of an assignment statement showing the use of an index:

```
RainFall(1)=3.1
```

We saw earlier that we could use the DIMENSION attribute to indicate that a variable was an array. In the above example Fortran statement our array is called RainFall. In this statement we are assigning the value 10.4 to the first element of the array; i.e., the rainfall for the month of January is 10.4. We use the index 1 to represent the first month. Consider the following statement:

```
SummerAverage = (RainFall(6) + RainFall(7) + &
                 RainFall(8))/3
```

This statement says take the values of the rainfall for June, July and August, add them up and then divide by 3, and assign the result to the variable SummerAverage, thus providing us with the rainfall average for the three summer months — Northern Hemisphere of course.

9.6.1 Example 1: Rainfall

The following program reads in the 12 monthly values from the terminal, computes the sum and average for the year, and prints the average out.

```
PROGRAM ch0901
IMPLICIT NONE
REAL :: Total=0.0, Average=0.0
REAL , DIMENSION(1:12) :: RainFall
INTEGER :: Month
  PRINT *,' Type in the rainfall values'
  PRINT *,' one per line'
  DO Month=1,12
    READ *, RainFall(Month)
  ENDDO
  DO Month=1,12
    Total = Total + RainFall(Month)
  ENDDO
  Average = Total / 12
  PRINT *,' Average monthly rainfall was'
  PRINT *, Average
END PROGRAM ch0901
```

RainFall is the *array name*. The variable Month in brackets is the index. It takes on values from 1 to 12 inclusive, and is used to pick out or select elements of the

array. The index is thus a variable and this permits dynamic manipulation of the array at *run time*. The general form of the DO statement is

```
DO Counter = Start, End, Increment
```

The block of statements that form the loop is contained between the DO statement, which marks the beginning of the block or loop, and the ENDDO statement, which marks the end of the block or loop.

In this program, the DO loops take the form:

```
DO Month=1,12          start
   ...                       body
ENDDO                  end
```

The body of the loop in the program above has been indented. This is *not* required by Fortran. However it is good practice and will make programs easier to follow.

The number of times that the DO loop is executed is governed by the last part of the DO statement, i.e., by the

```
Counter = Start, End, Increment
```

Start as it implies, is the initial value which the counter (or index, or control variable) takes. Each time the loop is executed, the value of the counter will be increased by the value of *increment,* until the value of *end* is reached. If *increment* is omitted, it is assumed to be 1. No other element of the DO statement may be omitted. In order to execute the statements within the loop (the *body*) it must be possible to reach *end* from *start.* Thus zero is an illegal value of *increment*. In the event that it is not possible to reach *end,* the loop will not be executed and control will pass to the statement after the end of the loop.

In the example above, both loops would be executed 12 times. In both cases, the first time around the loop the variable MONTH would have the value 1, the second time around the loop the variable MONTH would have the value 2, etc., and the last time around the loop MONTH would have the value 12.

9.7 People's weights

In the table below we have ten people, with their names as shown. We associate each name with a number — in this case we have ordered the names alphabetically, and the numbers therefore reflect their ordering. WEIGHT is the *array name*. The number in brackets is called the *index* and it is used to pick out or select elements of the array. The table is read as the first element of the array WEIGHT has the value 85, the second element has the value 76*, etc.*

Person	Associated integer representation	Array and index	Associated value
Andy	1	Weight(1)	85
Barry	2	Weight(2)	76
Cathy	3	Weight(3)	85
Dawn	4	Weight(4)	90
Elaine	5	Weight(5)	69
Frank	6	Weight(6)	83
Gordon	7	Weight(7)	64
Hannah	8	Weight(8)	57
Ian	9	Weight(9)	65
Jatinda	10	Weight(10)	76

9.7.1 Example 2: Setting array size with a parameter

In the first example we so-called *hard coded* the number 12, which is the number of months, into the program. It occurred four times. Modifying the program to work with a different number of months would obviously be tedious and potentially error prone.

In this example we parameterise the size of the array and reduce the effort involved in modifying the program to work with a different number of people:

```
PROGRAM ch0902
! The program reads up to number_of_people weights
! into the array Weight
! Variables used
! Weight, holds the weight of the people
! Person, an index into the array
! Total, total weight
! Average, average weight of the people
! Parameters used
! NumberOfPeople ,10 in this case.
! The weights are written out so that
! they can be checked
!
IMPLICIT NONE
INTEGER , PARAMETER :: Number_Of_People = 10
REAL ::  Total = 0.0, Average = 0.0
```

```
INTEGER :: Person
REAL , DIMENSION(1:Number_of_People) :: Weight
  DO Person=1,Number_Of_People
    PRINT *, ' Type in the weight for person ',Person
    READ *,Weight(Person)
    Total = Total + Weight(Person)
  ENDDO
  Average = Total / Number_Of_People
  PRINT *,' The total of the weights is ',Total
  PRINT *,' Average Weight is ',Average
  PRINT *,' ',Number_of_People,' Weights were '
  DO Person=1,Number_Of_People
    PRINT *,Weight(Person)
  ENDDO
END PROGRAM ch0902
```

9.8 Summary

The DIMENSION attribute declares a variable to be an array, and must come at the start of a program unit, with other *declarative* statements. It has two forms and examples of both of them are given below. In the first case we explicitly specify the upper and lower limts:

```
REAL , DIMENSION(1:Number_of_People) :: Weight
```

In the second case the lower limit defaults to 1

```
REAL , DIMENSION(Number_of_People) :: Weight
```

The latter form will be seen in legacy code, especially Fortran 77 code suites.

The PARAMETER attribute declares a variable to have a fixed value that cannot be changed during the execution of a program. In our example above note that this statement occurs before the other declarative statements that depend on it. To recap the statements covered so far, the order is summarised below.

PROGRAM	First statement	
INTEGER REAL CHARACTER	*Declarative*	In any order and the DIMENSION and PARAMETER attributes are added here
Arithmetic assignment PRINT * READ * DO ENDDO	*Executable*	In any order
END PROGRAM	Last statement	

We choose individual members using an index, and these are always of integer type in Fortran.

The DO loop is a very convenient control structure for manipulating arrays, and we use indentation to clearly identify loops.

9.9 Problems

1. Compile and run examples 1 and 2 from this chapter.

2. Using a DO loop and an array rewrite the program which calculated the average of five numbers (Question 3 in Chapter 8) and increase the number of values read in from five to ten.

3.1 Modify the program that calculates the total and average of people's weights to additionally read in their heights and calculate the total and average of their heights. Use the data given below, which have been taken from a group of first year undergraduates:

```
Height      Weight
1.85           85
1.80           76
1.85           85
1.70           90
```

```
1.75          69
1.67          83
1.55          64
1.63          57
1.79          65
1.78          76
```

3.2 Your body mass index is given by your weight (in kilos) divided by your height (in metres) squared. Calculate and print out the BMI for each person.

Grades of obesity according to Garrow as follows:

Grade 0 (desirable) 20–24.9

Grade 1 (overweight) 25–29.9

Grade 2 (obese) 30–40

Grad 3 (morbidly obese) >40

Ideal BMI range,

Men, Range 20.1–25 kg/m^2

Women, Range 18.7–23.8 kg/m^2

3.3 When working on either a UNIX system or a PC in a DOS box it is possible to use the following characters to enable you to read data from a file or write output to a file when running your program:

Character	**Meaning**
<	read from file
>	write to file

On a typical UNIX system we could use

```
a.out < data.dat > results.txt
```

to read the data from the file called data.dat and write the output to a file called results.txt.

On a PC in a DOS box the equivalent would be

```
program.exe < data.dat > results.txt
```

This is a quick and dirty way of developing programs that do simple I/O; we don't have to keep typing in the data and we also have a record of the behaviour of the

program. Rerun the program that prints out the BMI values to write the output to a file called results.txt. Examine this file in an editor.

4. Modify the program that read in your name to read in ten names. Use an array and a DO loop. When you have read the names into the array write them out in reverse order on separate lines.

Hint: Look at the formal syntax of the DO statement.

5. Modify the rainfall program (which assumes that the measurement is in inches) to convert the values to centimetres. One inch equals 2.54 centimetres. Print out the two sets of values as a table.

Hint: Use a second array to hold the metric measurements.

6. Combine the programs that read in and calculate the average weight with the one that reads in peoples names. The program should read the weights into one array and the names into another. Allow 20 characters for the length of a name. Print out a table linking names and weights.

7. In an earlier chapter we used the following formula to calculate the period of a pendulum:

```
T = 2 * PI * (LENGTH / 9.81) ** .5
```

Write a program that uses a DO loop to make the length go from 1 to 10 metres in 1-metre increments.

Produce a table with two columns, the first of lengths and the second of periods.

10

Arrays 2
Further Examples

"Sir, In your otherwise beautiful poem (*The Vision of Sin*) there is a verse which reads
Every moment dies a man,
every moment one is born.
Obviously this cannot be true and I suggest that in the next edition you have it read
Every moment dies a man,
every moment 1 1/16 is born.
Even this value is slightly in error but should be sufficiently accurate for poetry."

Charles Babbage in a letter to Lord Tennyson

Aims

The aims of the chapter are to extend the concepts introduced in the previous chapter and in particular:

- To set an array size at run time - ALLOCATABLE arrays.
- To introduce the idea of an array with more than one dimension and the corresponding control structure to permit easy manipulation of higher-dimensioned arrays.
- To introduce an extended form of the DIMENSION attribute declaration, and the corresponding alternative form to the DO statement, to manipulate the array in this new form.
- To introduce the DO loop as a mechanism for the control of repetition in general, not just for manipulating arrays.
- To formally define the block DO syntax.

10 Arrays 2: Further Examples

10.1 Varying the array size at run time

The earlier examples set the array size in the following two ways:

- Explicitly using a numeric constant
- Implicitly using a parameterised variable

In both cases we knew the size of the array at the time we compiled the program. We may not know the size of the array at compile time and Fortran provides the ALLOCATABLE attribute to accommodate this kind of problem. Consider the following example.

```
PROGRAM ch1001
!
! This program is a simple variant of ch0902.
! The array is now allocatable
! and the user is prompted for the
! number of people at run time.
!
IMPLICIT NONE
INTEGER :: Number_Of_People
REAL ::  Total = 0.0, Average = 0.0
INTEGER :: Person
REAL , DIMENSION(:) , ALLOCATABLE :: Weight
   PRINT *,' How many people?'
   READ *,Number_Of_People
   ALLOCATE(Weight(1:Number_Of_People))
   DO Person=1,Number_Of_People
      PRINT *, ' Type in the weight for person ',Person
      READ *,Weight(Person)
      Total = Total + Weight(Person)
   ENDDO
   Average = Total / Number_Of_People
   PRINT *,' The total of the weights is ',Total
   PRINT *,' Average Weight is ',Average
   PRINT *,' ',Number_of_People,' Weights were '
   DO Person=1,Number_Of_People
      PRINT *,Weight(Person)
   ENDDO
END PROGRAM ch1001
```

The first statement of interest is the type declaration with the dimension and allocatable attributes, e.g.,

```
REAL , DIMENSION(:) , ALLOCATABLE :: Weight
```

The second is the ALLOCATE statement where the value of the variable Number_of_people is not known until run time, e.g.,

```
ALLOCATE(Weight(1:Number_Of_People))
```

We will look more formally at these statements in Chapter 11.

10.2 Higher-dimension arrays

There are many instances where it is necessary to have arrays with more than one dimension. Consider the examples below.

10.2.1 A map

Consider the representation of the height of an area of land expressed as a two-dimensional table of numbers e.g., we may have some information represented in a simple table as follows:

	Longitude		
Latitude	1	2	3
1	10.0	40.0	70.0
2	20.0	50.0	80.0
3	30.0	60.0	90.0

The values in the *array* are the heights above sea level. The example is obviously artificial, but it does highlight the concepts involved. For those who have forgotten their geography, lines of latitude run east–west (the equator is a line of latitude) and lines of longitude run north–south (they go through the poles and are all of the same length). In the above table therefore the latitude values are ordered by row and the longitude values are ordered by column.

A program to manipulate this data structure would involve something like the following:

```
PROGRAM C1002
! Variables used
! Height - used to hold the heights above sea level
! Long - used to represent the longitude
! Lat - used to represent the latitude
!    both restricted to integer values.
! Correct - holds the correction factor
IMPLICIT NONE
INTEGER , PARAMETER :: Size = 3
INTEGER  :: Lat , Long
REAL , DIMENSION(1:Size,1:Size) :: Height
REAL , PARAMETER :: Correct = 10.0
  DO Lat = 1,Size
    DO Long = 1,Size
      PRINT *,' Type in value at ',Lat,' ',Long
      READ * , Height(Lat,Long)
    ENDDO
  ENDDO
  DO Lat = 1,Size
    DO Long = 1,Size
      Height(Lat,Long) = Height(Lat,Long) + Correct
    ENDDO
  ENDDO
  PRINT * , ' Corrected data is '
  DO Lat = 1,Size
    DO Long = 1,Size
      PRINT * , Height(Lat,Long)
    ENDDO
  ENDDO
END PROGRAM C1002
```

Note the way in which indentation has been used to highlight the structure in this example. Note also the use of a textual prompt to highlight which data value is expected. Running the program highlights some of the problems with the simple I/O used in the example above. We will address this issue in the next example.

The *inner* loop is said to be *nested* within the outer one. It is very common to encounter problems where nesting is a natural way to express the solution. Nesting is permitted to any depth. Here is an example of a valid nested DO loop:

```
  DO              ! Start of outer loop
    DO               ! Start of inner loop
      .
```

```
        .
      ENDDO           ! End of inner loop
   ENDDO           ! End of outer loop
```

This example introduces the concept of two indices, and can be thought of as a row and column data structure.

10.2.2 Example 3: Sensible tabular output

The first example had the values printed in a format that wasn't very easy to work with. In this example we introduce a so-called implied DO loop, which enables us to produce neat and humanly comprehensible output:

```
PROGRAM C1003
! Variables used
! Height - used to hold the heights above sea level
! Long - used to represent the longitude
! Lat - used to represent the latitude
!     both restricted to integer values.
IMPLICIT NONE
INTEGER , PARAMETER :: Size = 3
INTEGER  :: Lat , Long
REAL , DIMENSION(1:Size,1:Size) :: Height
REAL , PARAMETER :: Correct = 10.0
  DO Lat = 1,Size
    DO Long = 1,Size
     READ * , Height(Lat,Long)
     Height(Lat,Long) = Height(Lat,Long) + Correct
    ENDDO
  ENDDO
  DO Lat = 1,Size
    PRINT * , (Height(Lat,Long),Long=1,3)
  ENDDO
END PROGRAM C1003
```

The key statement in this example is

```
PRINT * , (Height(Lat,Long),Long=1,3)
```

This is called an implied DO loop, as the longitude variable takes on values from 1 through 3 and will write out all three values on one line.

We will see other examples of this statement as we go on.

10.2.3 Example 4: Average of three sets of values

This example extends the previous one. Now we have three sets of measurements and we are interested in calculating the average of these three sets. The two new data sets are:

```
 9.5     39.5     69.5
19.5     49.5     79.5
29.5     59.5     89.5
```

and

```
10.5     40.5     70.5
20.5     50.5     80.5
30.5     60.5     90.5
```

and we have chosen the values to enable us to quickly check that the calculations for the averages are correct.

This program also uses implied DO loops to read the data, as data in files are generally tabular:

```
PROGRAM C1004
! Variables used
! H1,H2,H3 - used to hold the heights above sea level
! H4 - used to hold the average of the above
! Long - used to represent the longitude
! Lat - used to represent the latitude
!    both restricted to integer values.
IMPLICIT NONE
INTEGER , PARAMETER :: Size = 3
INTEGER  :: Lat , Long
REAL , DIMENSION(1:Size,1:Size) :: H1,H2,H3,H4
  DO Lat = 1,Size
       READ * , (H1(Lat,Long), Long=1,Size)
  ENDDO
  DO Lat = 1,Size
       READ * , (H2(Lat,Long), Long=1,Size)
  ENDDO
  DO Lat = 1,Size
       READ * , (H3(Lat,Long), Long=1,Size)
  ENDDO
  DO Lat = 1,Size
    DO Long = 1,Size
      H4(Lat,Long)=( H1(Lat,Long) + H2(Lat,Long) + &
```

```
                    H3(Lat,Long) ) / Size
     ENDDO
   ENDDO
   DO Lat = 1,Size
        PRINT * , (H4(Lat,Long),Long=1,3)
   ENDDO
END PROGRAM C1004
```

The original data was accurate to three significant figures. The output from the above has spurious additional accuracy. We will look at how to correct this in the later chapter on output.

10.2.4 Example 5: Booking arrangements in a theatre or cinema

A theatre or cinema consists of rows and columns of seats. In a large cinema or a typical theatre there would also be more than one level or storey. Thus, a program to represent and manipulate this structure would probably have a two-d or three-d array. Consider the following program extract:

```
PROGRAM ch1005
IMPLICIT NONE
INTEGER   , PARAMETER :: NR=5
INTEGER   , PARAMETER :: NC=10
INTEGER   , PARAMETER :: NF=3
INTEGER :: Row,Column,Floor
CHARACTER*1 , DIMENSION(1:NR,1:NC,1:NF) :: Seats=' '
   DO   Floor=1,NF
     DO   Row=1,NR
       READ *,(Seats(Row,Column,Floor),Column=1,NC)
     ENDDO
   ENDDO
   PRINT *,' Seat plan is'
   DO   Floor=1,NF
     PRINT *,' Floor = ',Floor
     DO   Row=1,NR
       PRINT *,(Seats(Row,Column,Floor),Column=1,NC)
     ENDDO
   ENDDO
END PROGRAM ch1005
```

Note here the use of the term PARAMETER in conjunction with the INTEGER declaration. This is called an entity orientated declaration. An alternative to this is an attribute-orientated declaration, e.g.,

```
INTEGER :: NR,NC,NF
PARAMETER :: NR=5,NC=10,NF=3
```

and we will be using the entity-orientated declaration method throughout the rest of the book. This is our recommended method as you only have to look in one place to determine everything that you need to know about an entity.

10.3 Additional forms of the DIMENSION attribute and DO loop statement

10.3.1 Example 6: Voltage from –20 to +20 volts

Consider the problem of an experiment where the independent variable voltage varies from –20 to +20 volts and the current is measured at 1-volt intervals. Fortran has a mechanism for handling this type of problem:

```
PROGRAM C1006
IMPLICIT NONE
REAL , DIMENSION(-20:20) :: Current
REAL :: Resistance
INTEGER :: Voltage
  PRINT *,' Type in the resistance'
  READ *, Resistance
  DO  Voltage = -20,20
    Current(Voltage)=Voltage/Resistance
    PRINT *, Voltage, ' ', Current(Voltage)
  ENDDO
END PROGRAM C1006
```

We appreciate that, due to experimental error, the voltage will not have exact integer values. However, we are interested in representing and manipulating a set of values, and thus from the point of view of the problem solution and the program this is a reasonable assumption. There are several things to note.

This form of the DIMENSION attribute

```
DIMENSION(First:Last)
```

is of considerable use when the problem has an effective index which does not start at 1.

There is a corresponding form of the DO statement which allows processing of problems of this nature. This is shown in the above program. The general form of the DO statement is therefore:

```
   DO counter=start, end, increment
```

where *start, end* and *increment* can be positive or negative. Note that zero is a legitimate value of the dimension limits and of a DO loop index.

10.3.2 Example 7: Longitude from –180 to +180

Consider the problem of the production of a table linking time difference with longitude. The values of longitude will vary from –180 to +180 degrees, and the time will vary from +12 hours to –12 hours. A possible program segment is:

```
PROGRAM ch1007
IMPLICIT NONE
REAL , DIMENSION(-180:180) :: Time=0
INTEGER :: Degree,Strip
REAL :: Value
  DO Degree=-180,165,15
    Value=Degree/15.
    DO Strip=0,14
      Time(Degree+Strip)=Value
    ENDDO
  ENDDO
  DO Degree=-180,180
    PRINT *,Degree,' ',Time(Degree)
  END DO
END PROGRAM ch1007
```

10.3.3 Notes

The values of the time are **not** being calculated at every degree interval.

The variable Time is a real variable. It would be possible to arrange for the time to be an integer by expressing it in either minutes or seconds.

This example takes no account of all the wiggly bits separating time zones or of British Summer Time.

What changes would you make to the program to accommodate +180? What is the time at –180 and +180?

10.4 The DO loop and straight repetition

10.4.1 Example 8: Table of temperatures

Consider the production of a table of liquid measurements. The independent variable is the litre value; the gallon and US gallon are the dependent variables. Strictly speaking, a program to do this does not have to have an array, i.e., the DO

loop can be used to control the repetition of a set of statements that make no reference to an array. The following shows a complete but simple conversion program:

```
PROGRAM ch1008
IMPLICIT NONE
!
! 1 us gallon = 3.7854118 litres
! 1 uk gallon = 4.545      litres
!
INTEGER :: Litre
REAL    :: Gallon,USGallon
  DO Litre = 1,10
    Gallon   = Litre * 0.2641925
    USGallon = Litre * 0.220022
    PRINT *,Litre, ' ',Gallon,' ',USGallon
  END DO
END PROGRAM ch1008
```

Note here that the DO statement has been used *only* to control the repetition of a block of statements — there are no arrays at all in this program.

This is the other use of the DO statement. The DO loop thus has two functions — its use with arrays as a control structure and its use solely for the repetition of a block of statements.

10.4.2 Example 9: Means and standard deviations

In the calculation of the mean and standard deviation of a list of numbers, we can use the following formulae. It is not actually necessary to store the values, nor to accumulate the sum of the values and their squares. In the first case, we would possibly require a large array, whereas in the second, it is conceivable that the accumulated values (especially of the squares) might be too large for the machine. The following example uses an *updating* technique which avoids these problems, but is still accurate. The DO loop is simply a control structure to ensure that all the values are read in, with the index being used in the calculation of the updates:

```
PROGRAM ch1009
! Variables used are
!     Mean - for the running mean
!     SSQ  - The running corrected sum of squares
!     X    - Input values for which
! mean and sd required
!     W    - Local work variable
!     SD   - Standard Deviation
!     R    - Another work variable
```

```
IMPLICIT NONE
REAL :: Mean=0.0,SSQ=0.0,X,W,SD,R
INTEGER :: I,N
   PRINT *,' ENTER THE NUMBER OF READINGS'
   READ*,N
   PRINT*,' ENTER THE ',N,' VALUES, ONE PER LINE'
   DO I=1,N
      READ*,X
      W=X-Mean
      R=I-1
      Mean=(R*Mean+X)/I
      SSQ=SSQ+W*W*R/I
   ENDDO
   SD=(SSQ/R)**0.5
   PRINT *,' Mean is ',Mean
   PRINT *,' Standard deviation is ',SD
END PROGRAM ch1009
```

10.5 Summary

Arrays can have up to seven dimensions.

DO loops may be nested, but they must not overlap.

The DIMENSION attribute allows limits to be specified for a block of information which is to be treated in a common way. The limits must be integer, and the second limit must exceed the first, e.g.,

```
   REAL , DIMENSION(-123:-10) :: List
   REAL , DIMENSION(0:100,0:100) :: Surface
   REAL , DIMENSION(1:100) :: Value
```

The last example could equally be written

```
   REAL , DIMENSION(100) :: Value
```

where the first limit is omitted and is given the default value 1. The array LIST would contain 114 values, while Surface would contain 10201.

A DO statement and its corresponding ENDDO statement define a loop. The DO statement provides a starting value, terminal value, and optionally, an increment for its index or counter.

The increment may be negative, but should never be zero. If it is not present, the default value is 1. It must be possible for the terminating value to be reached from the starting value.

The counter in a DO loop is ideally suited for indexing an array, but it may be used anywhere that repetition is needed, and of course the index or counter need not be used explicitly.

The formal syntax of the block DO construct is

```
[ do-construct-name : ] DO [label] [ loop-control ]
   [execution-part-construct ]
[ label ] end-do
```

where the forms of the loop control are

```
[ , ] scalar-variable-name =
scalar-numeric-expression ,
scalar-numeric-expression
[ , scalar-numeric-expression ]
```

and the forms of the end-do are

```
END DO [ do-construct-name ]
CONTINUE
```

and [] identify optional components of the block DO construct. This statement is looked at in much greater depth in Chapter 16.

10.6 Problems

1. Compile and run all the examples in this chapter, except example 5. This is covered separately later.

2. Modify the first example to convert the height in feet to height in metres. The conversion factor is one 1 equals 0.305 metres.

Hint: You can either overwrite the height array or introduce a second array.

3. The following are two equations for temperature conversion

c = 5 /9 * (t-32)

f = 32 + 9 /5 * t

Write a complete program where t is an integer DO loop variable and loop from −50 to 250. Print out the values of c, t and f on one line. What do you notice about the c and f values?

4. Write a program to print out the 12 times table. Typical output would be of the form:

1 * 12 = 12

2 * 12 = 24

3 * 12 = 36

etc.

Hint: You don't need to use an array here.

5. Write a program to read the following data into a two-dimensional array:

1 2 3
4 5 6
7 8 9

Calculate totals for each row and column and produce an output similar to that below:

1 2 3 6
4 5 6 15
7 8 9 24
12 15 18

Hint 1: Example ch0902 shows how to sum over a loop.

Hint 2: You need to introduce two one-dimensional arrays to hold the row and column totals. You need to index over the rows to get the column totals and over the columns to get the row totals.

6. Modify the above to produce averages for each row and column as well as the totals.

9. Using the following data from Problem 2 in Chapter 9:

```
1.85    85
1.80    76
1.85    85
1.70    90
1.75    69
1.67    83
1.55    64
1.63    57
1.79    65
1.78    76
```

Use the program that evaluated the mean and standard deviation to do so for these heights and weights.

In the first case use the program as is and run it twice, first with the heights then with the weights.

What changes would you need to make to the program to read a height and a weight in a pair?

Hint: You could introduce separate scalar variables for the heights and weights.

10. Example 5 looked at seat bookings in a cinema or theatre. Here is an example of a sample data file for this program

```
P  P  P  P  P  P  P  P  P  P
P  P  P  C  C  C  C  P  P  P
C  C  C  E  E  P  P  P  P  P
C  C  C  C  C  C  C  C  C  C
E  E  E  P  P  P  P  P  P  P
C  C  E  E  P  P  C  C  E  E
P  P  P  P  P  P  P  P  P  P
P  P  P  C  C  C  C  P  P  P
C  C  C  E  E  P  P  P  P  P
C  C  C  C  C  C  C  C  C  C
E  E  E  P  P  P  P  P  P  P
C  C  E  E  P  P  C  C  E  E
P  P  P  P  P  P  P  P  P  P
P  P  P  C  C  C  C  P  P  P
C  C  C  E  E  P  P  P  P  P
```

The key for this is as follows:

C = Confirmed Booking

P = Provisional Booking

E = Seat Empty

Compile and run the program. The output would benefit from adding row and column numbers to the information displayed. We will come back to this issue in a subsequent chapter on output formatting.

The data are in a file on the web and the address is given below.

- http://www.kcl.ac.uk/fortran

Problem 3.3 in the last chapter shows how to read data from a file.

11

Whole Array and Additional Array Features

"A good notation has a subtlety and suggestiveness which at times make it seem almost like a live teacher."

Bertrand Russell

Aims

The aims of the chapter are:

- To look more formally at the terminology required to precisely describe arrays.
- To introduce ways in which we can manipulate whole arrays and parts of arrays (sections).
- ALLOCATABLE arrays — ways in which the size of an array can be deferred until execution time.
- To introduce the concept of array element ordering and physical and virtual memory.
- To introduce ways in which we can initialise arrays using array constructors.
- To introduce the WHERE statement and array masking.
- To introduce the FORALL statement and construct.

11 Whole Array and Additional Array Features

11.1 Terminology

Fortran supports an abundance of array handling features. In order to make the description of these features more precise a number of additional terms have to be covered and these are introduced and explained below.

11.1.1 Rank

The number of dimensions of an array is called its rank. A one-dimensional array has rank 1, a two-dimensional array has rank 2 and so on.

11.1.2 Bounds

An array's bounds are the upper and lower limits of the index in each dimension.

11.1.3 Extent

The number of elements along a dimension of an array is called the extent.

```
INTEGER, DIMENSION(-10:15):: Current
```

has bounds –10 and 15 and an extent of 26.

11.1.4 Size

The total number of elements in an array is its size.

11.1.5 Shape

The shape of an array is determined by its rank and its extents in each dimension.

11.1.6 Conformable

Two arrays are said to be conformable if they have the same shape, that is, they have the same rank and the same extent in each dimension.

11.1.7 Array element ordering

Array element ordering states that the elements of an array, regardless of rank, form a linear sequence. The sequence is such that the subscripts along the first dimension vary most rapidly, and those along the last dimension vary most slowly. This is best illustrated by considering, for example, a rank 2 array A defined by

```
REAL , DIMENSION(1:4,1:2) :: A
```

A has 8 real elements whose array element order is

A(1,1), A(2,1), A(3,1), A(4,1), A(1,2), A(2,2), A(3,2), A(4,2)

i.e., mathematically by column and not row.

11.2 Whole array manipulation

The examples of arrays so far have shown operations on arrays via array elements. One of the significant features of Fortran is its ability to manipulate arrays as whole objects. This allows arrays to be referenced not just as single elements but also as groups of elements. Along with this ability comes a whole host of intrinsic procedures for array processing. These procedures are mentioned in Chapter 14, and listed in alphabetical order with examples in Appendix D.

11.2.1 Assignment

An array name without any indices can appear on both sides of assignment and input and output statements. For example, values can be assigned to all the elements of an array in one statement:

```
REAL, DIMENSION(1:12):: Rainfall
Rainfall=0.0
```

The elements of one array can be assigned to another:

```
INTEGER, DIMENSION(1:50) :: A,B
...
A=B
```

Arrays A and B must be conformable in order to do this.

The following example is **illegal** since X is rank 1 and extent 20, whilst Z is rank 1 and extent 41.

```
REAL, DIMENSION(1:20) :: X
REAL, DIMENSION(1:41) :: Z
X=50.0
Z=X
```

But the following is legal because both arrays are now conformable, i.e., they are both of rank 1 and extent 41:

```
REAL , DIMENSION (-20:20) :: X
REAL , DIMENSION (1:41) :: Y
X=50.0
Y=X
```

11.2.2 Expressions

All the arithmetic operators available to scalars are available to arrays, but care must be taken because mathematically they may not make sense.

```
REAL , DIMENSION (1:50) :: A,B,C,D,E
C=A+B
```

adds each element of A to the corresponding element of B and assigns the result to C.

```
E=C*D
```

multiplies each element of C by the corresponding element of D. This is **not** vector multiplication. To perform a vector dot product there is an intrinsic procedure DOT_PRODUCT, and an example of this is given in a subsequent section on array constructors.

For higher dimensions

```
REAL ,DIMENSION (1:10,1:10) :: F,G,H
F=F**0.5
```

takes the square root of every element of F.

```
H=F+G
```

adds each element of F to the corresponding element of G.

```
H=F*G
```

multiplies each element of F by the corresponding element of G. The last statement is **not** matrix multiplication. An intrinsic procedure MATMUL performs matrix multiplication; further details are given in Appendix D.

Consider the following example, which is a solution to a problem set earlier, but is now addressed using some of the whole array features of Fortran

```
PROGRAM ch1101
IMPLICIT NONE
INTEGER , PARAMETER :: N=12
REAL , DIMENSION(1:N) :: RainFall_ins=0.0
REAL , DIMENSION(1:N) :: RainFall_cms=0.0
INTEGER :: Month
   PRINT *, ' Input the rainfall values in inches'
   READ *, RainFall_ins
   RainFall_cms=RainFall_ins * 2.54
   DO Month=1,N
      PRINT * , ' ', Month , ' ' , &
                     RainFall_ins(Month) , ' ' , &
                     RainFall_cms(Month)
```

```
   END DO
END PROGRAM ch1101
```

The statements

```
REAL , DIMENSION(1:N) :: RainFall_ins=0.0
REAL , DIMENSION(1:N) :: RainFall_cms=0.0
```

are examples of whole array initialisation. Each element of the arrays is set to 0.0.

The statement

```
   READ *, RainFall_ins
```

is an example of whole array I/O, where we no longer have to use a DO loop to read each element in.

Finally, we have the statement

```
   RainFall_cms = RainFall_ins * 2.54
```

which is an example of whole array arithmetic and assignment.

Here is a two-dimensional example:

```
PROGRAM ch1102
! This program reads in a grid of temperatures
! (degrees Fahrenheit) at 25 grid references
! and converts them to degrees Celsius
IMPLICIT NONE
REAL, DIMENSION (1:5,1:5) :: Fahrenheit, Celsius
INTEGER :: Long, Lat
!
! Read in the temperatures
!
   DO Lat=1,5
      PRINT *, ' For Latitude= ',Lat
      DO Long=1,5
         PRINT *, ' For Longitude', Long
         READ *,Fahrenheit( Long, Lat)
      END DO
   END DO
!
! Conversion applied to all values
!
   Celsius = 5.0/9.0 * (Fahrenheit - 32.0)
```

```
   PRINT * , Celsius
   PRINT * , Fahrenheit
END PROGRAM ch1102
```

Note the use of whole arrays in the print statements. The output does look rather messy though, and also illustrates array element ordering.

11.3 Array sections

Often it is necessary to access part of an array rather than the whole, and this is possible with Fortran's powerful array manipulation features.

11.3.1 Rank 1 array example

Consider the following:

```
program ch1103
implicit none
integer , dimension(-5:5) :: x
integer :: i
   x(-5:-1) = -1
   x(0)      =  0
   x(1:5)    =  1
   do i=-5,5
      print *,' ',i,' ',x(i)
   end do
end program ch1103
```

The statement

```
   x(-5:-1) = -1
```

is working with a section of an array. It assigns the value –1 to elements x(–5) through x(–1).

The statement

```
   x(1:5)    =  1
```

is also working with an array section. It assignes the value 1 to elements x(1) through x(5).

11.3.2 Rank 2 array example

In Chapter 9 we gave an example of a table of examination marks, and this is given again below:

Name	Physics	Maths	Biology	History	English	French
Fowler L.	50	47	28	89	30	46
Barron L.W	37	67	34	65	68	98
Warren J.	25	45	26	48	10	36
Mallory D.	89	56	33	45	30	65
Codd S.	68	78	38	76	98	65

The following program reads the data in, scales column 3 by 2.5 as the Biology marks were out of 40 (the rest are out of 100), calculates the averages for each subject and for each person and prints out the results.

```
program ch1104
implicit none
integer , parameter :: nrow=5
integer , parameter :: ncol=6
REAL , DIMENSION(1:nrow,1:ncol) &
                        :: Exam_Results     = 0.0
real , dimension(1:nrow) &
                        :: People_average   = 0.0
real , dimension(1:ncol) &
                        :: Subject_Average = 0.0
integer :: r,c
  do r=1,nrow
    read *, exam_results(r,1:ncol)
  end do
  Exam_Results(1:nrow,3) = 2.5 * Exam_Results(1:nrow,3)
  do r=1,nrow
    do c=1,ncol
      people_average(r) = people_average(r) + &
                          exam_results(r,c)
    end do
  end do
  people_average = people_average / ncol
  do c=1,ncol
    do r=1,nrow
      subject_average(c) = subject_average(c) + &
                           exam_results(r,c)
    end do
```

```
   end do
   subject_average = subject_average / nrow
   print *,' People averages'
   print *, people_average
   print *, ' Subject averages'
   print *, subject_average
end program ch1104
```

The statement

```
     read *, exam_results(r,1:ncol)
```

uses sections to replace the implied DO loop in the earlier example.

The statement

```
   Exam_Results(1:nrow,3) = 2.5 * Exam_Results(1:nrow,3)
```

uses array sections in the arithmetic and the assignment.

11.4 Array constructors

Arrays can be given intial values in Fortran using array constructors. Some examples are given below.

11.4.1 Rank 1 array example — explicit values

```
PROGRAM ch1105
IMPLICIT NONE
integer :: n=12
REAL :: Total=0.0, Average=0.0
REAL , DIMENSION(1:n) :: RainFall = &
   (/3.1,2.0,2.4,2.1,2.2,2.2,1.8,2.2,2.7,2.9,3.1,3.1/)
INTEGER :: Month
   DO Month=1,n
      Total = Total + RainFall(Month)
   ENDDO
   Average = Total / n
   PRINT *,' Average monthly rainfall was'
   PRINT *, Average
END PROGRAM ch1105
```

The statement

```
REAL , DIMENSION(1:n) :: RainFall = &
   (/3.1,2.0,2.4,2.1,2.2,2.2,1.8,2.2,2.7,2.9,3.1,3.1/)
```

provides initial values to the elements of the array Rainfall.

11.4.1.1 Rank 1 array example and implied DO loop

The next example uses a simple variant:

```
PROGRAM ch1106
IMPLICIT NONE
!
! 1 us gallon = 3.7854118 litres
! 1 uk gallon = 4.545      litres
!
integer , parameter :: n=10
integer :: i
INTEGER , dimension(1:n) :: Litre=(/(i,i=1,n)/)
REAL    , dimension(1:n) :: Gallon,USGallon
  Gallon    = Litre * 0.2641925
  USGallon = Litre * 0.220022
  DO i = 1,n
     PRINT *,Litre(i), ' ',Gallon(i),' ',USGallon(i)
  END DO
END PROGRAM ch1106
```

The statement

```
INTEGER , dimension(1:n) :: Litre=(/(i,i=1,n)/)
```

initialises the 10 elements of the Litre array to the values 1,2,3,4,5,6,7,8,9,10 respectively.

11.4.1.2 Rank 1 array example and the DOT_PRODUCT intrinsic

The following example uses an array constructor and the intrinsic procedure DOT_PRODUCT:

```
INTEGER , DIMENSION(1:3) :: X,Y
INTEGER :: Result
X=(/1,3,5/)
Y=(/2,4,6/)
Result=DOT_PRODUCT(X,Y)
```

and Result has the value 44, which is obtained by the normal mathematical dot product operation, 1*2 + 3*4 + 5*6.

The general form of the array constructor is (/ a list of expressions/) where each expression is of the same type.

To construct arrays of higher rank than one the intrinsic function RESHAPE must be used. An introduction to intrinsic functions is given in Chapter 14, and an alphabetic list with a full explanation of each function is given in Appendix D. To use it in its simplest form:

Matrix = RESHAPE (Source, Shape)

where Source is a rank 1 array containing the values of the elements required in the new array, Matrix, and Shape is a rank 1 array containing the shape of the new array Matrix.

We consider the rank 1 array B=(1,3,5,7,9,11), and we wish to store these values in a rank 2 array A, such that A is the matrix:

$$A = \begin{pmatrix} 1 & 7 \\ 3 & 9 \\ 5 & 11 \end{pmatrix}$$

The following code extract is needed:

```
INTEGER, DIMENSION(1:6) :: B
INTEGER, DIMENSION(1:3, 1:2) :: A
B = (/1,3,5,7,9,11/)
A = RESHAPE(B,(/3,2/))
```

Note that the elements of the source array B must be stored in the array element order of the required array A.

The following example illustrates the additional forms of the RESHAPE function that are used when the number of elements in the source array is less than the number of elements in the destination. The complete form is

RESHAPE(Source, Shape, *Pad, Order)*

Pad and Order are optional. See Appendix D for a complete explanation of *Pad* and *Order*:

```
program ch1107
implicit none
integer , dimension(1:2,1:4) :: x
integer , dimension(1:8)    :: y=(/1,2,3,4,5,6,7,8/)
integer , dimension(1:6)    :: z=(/1,2,3,4,5,6/)
integer :: r,c
  print *,' Source array y'
  print *,y
  print *,' Source array z'
```

```
  print *,z
  print *,' Simple reshape sizes match'
  x=reshape(y,(/2,4/))
  do r=1,2
    print *,(x(r,c),c=1,4)
  end do
  print *,' Source 2 elements smaller pad with 0'
  x=reshape(z,(/2,4/),(/0,0/))
  do r=1,2
    print *,(x(r,c),c=1,4)
  end do
  print *,' As previous now specify order as 1*2'
  x=reshape(z,(/2,4/),(/0,0/),(/1,2/))
  do r=1,2
    print *,(x(r,c),c=1,4)
  end do
  print *,' As previous now specify order as 2*1'
  x=reshape(z,(/2,4/),(/0,0/),(/2,1/))
  do r=1,2
    print *,(x(r,c),c=1,4)
  end do
end program ch1107
```

11.4.2 Rank 1 example with step size of 2 in implied DO loop

Consider the following example:

```
program ch1108
implicit none
integer :: i
integer , dimension(1:10) :: x=(/(i,i=1,10)/)
integer , dimension(1:5)  :: odd=(/(i,i=1,10,2)/)
integer , dimension(1:5)  :: even
  even=x(2:10:2)
  print *,' x'
  print *,x
  print *,' odd'
  print *,odd
  print *,' even'
  print *,even
end program ch1108
```

The statement

```
integer , dimension(1:5)   :: odd=(/(i,i=1,10,2)/)
```

steps through the array 2 at a time.

The statement

```
   even=x(2:10:2)
```

shows an array section where we go from elements two through ten in steps of two. The 2:10:2 is an example of a subscript triplet in Fortran, and the first 2 is the lower bound, the 10 is the upper bound, and the last 2 is the increment. Fortran uses the term stride to mean the increment in a subscript triplet.

11.4.3 Rank 1 array and the SUM intrinsic function

The following example is based on ch1105. It uses the SUM intrinsic to calculate the sum of all the values in the Rainfall array.

```
PROGRAM ch1109
IMPLICIT NONE
REAL :: Total=0.0, Average=0.0
REAL , DIMENSION(12) :: RainFall = &
   (/3.1,2.0,2.4,2.1,2.2,2.2,1.8,2.2,2.7,2.9,3.1,3.1/)
INTEGER :: Month
   Total = SUM(RainFall)
   Average = Total / 12
   PRINT *,' Average monthly rainfall was'
   PRINT *, Average
END PROGRAM ch1109
```

The statement

```
   Total = SUM(RainFall)
```

replaces the statements below from the earlier example

```
   DO Month=1,n
      Total = Total + RainFall(Month)
   ENDDO
```

In this example SUM adds up all of the elements of the array Rainfall.

So we have three ways of processing arrays:

- Element by element.

- Using sections.
- On a whole array basis.

The ability to use sections and whole arrays when programming is a major advance of the element by element processing supported by Fortran 77.

11.4.4 Rank 2 arrays and the SUM intrinsic function

This example is based on the earlier exam results program:

```
program ch1110
implicit none
integer , parameter :: nrow=5
integer , parameter :: ncol=6
real , dimension(1:nrow*ncol)    :: results = &
                 (/50 , 47 , 28 , 89 , 30 , 46 , &
                   37 , 67 , 34 , 65 , 68 , 98 , &
                   25 , 45 , 26 , 48 , 10 , 36 , &
                   89 , 56 , 33 , 45 , 30 , 65 , &
                   68 , 78 , 38 , 76 , 98 , 65/)
REAL , DIMENSION(1:nrow,1:ncol) :: Exam_Results &
    = 0.0
real , dimension(1:nrow)        :: People_average &
    = 0.0
real , dimension(1:ncol)         :: Subject_Average &
    = 0.0
integer :: r,c
  exam_results = &
    reshape(results,(/nrow,ncol/),(/0.0,0.0/),(/2,1/))
  Exam_Results(1:nrow,3) = 2.5 * Exam_Results(1:nrow,3)
  subject_average = sum(exam_results,dim=1)
  people_average  = sum(exam_results,dim=2)
  people_average  = people_average  / ncol
  subject_average = subject_average / nrow
  print *,' People averages'
  print *, people_average
  print *, ' Subject averages'
  print *, subject_average
end program ch1110
```

This example has several interesting array features:

- We initialise a rank 1 array with the values we want in our exam marks array. The data are laid out in the program as they would be in an external file in rows and colums.
- We use RESHAPE to initialise our exam marks array. We use the fourth parameter (/2,1/) to populate the rank 2 array with the data in row order.
- We use SUM with a DIM of 1 to compute the sums for the subjects.
- We use SUM with a DIM of 2 to compute the sums for the people.

11.5 Masked array assignment and the WHERE statement

Fortran has array assignment both on an element by element basis and on a whole array basis. There is an additional form of assignment based on the concept of a logical mask.

Consider the example of time zones given in Chapter 10. The `Time` array will have values that are both negative and positive. We can then associate the positive values with the concept of east of the Greenwich meridian, and the negative values with the concept of west of the Greenwich meridian e.g.:

```
PROGRAM ch1111
IMPLICIT NONE
REAL , DIMENSION(-180:180) :: Time=0
INTEGER :: Degree,Strip
REAL :: Value
CHARACTER (LEN=1) , DIMENSION(-180:180) &
     :: Direction=' '
   DO Degree=-180,165,15
     Value=Degree/15.
     DO Strip=0,14
       Time(Degree+Strip)=Value
     ENDDO
   ENDDO
   DO Degree=-180,180
     PRINT *,Degree,' ',Time(Degree)
   END DO
   WHERE (Time > 0.0)
     Direction='E'
   ELSEWHERE (Time < 0.0)
     Direction='W'
   ENDWHERE
   PRINT *,direction
END PROGRAM ch1111
```

11.5.1 Notes

The arrays must be conformable, i.e., in our example Time and Direction are the same shape.

The selective assignment is achieved through the WHERE statement.

Both the WHERE and ELSEWHERE blocks can be executed.

The formal syntax is:

```
WHERE (array logical assignment)
   array assignment block
ELSEWHERE
   array assignment block
END WHERE
```

The first array assignment is executed where Time is positive and the is executed where Time is negative. For further coverage of logical expressions see Chapters 15 and 18.

11.6 The FORALL statement and FORALL construct

The FORALL statement and FORALL construct were introduced into Fortran to keep it inline with High Performance Fortran — HPF. They indicate to the compiler that the code can be optimised on a parallel processor. Consider the following example where a value is subtracted from the diagonal elements of a square matrix A:

```
FORALL (I=1:N)
  A(I,I) = A(I,I) - Lamda
END FORALL
```

The FORALL construct allows the calculations to be carried out simultaneously in a multiprocessor environment.

11.6.1 Syntax

```
FORALL ( triplet  [ , triplet ] ... [ , mask ] )
variable = expression
FORALL ( triplet  [ , triplet ] ... [ , mask ] )
pointer => target
```

The triplet specifies a value set for an index variable. It has the following syntax:

```
index = first : last [ : stride ]
```

First, last and stride are scalar integer expressions.

Mask is a scalar logical expression:

```
[ name : ] FORALL ( triplet [ , triplet ] ... [ ,
mask ] )
...
END FORALL [ name ]
```

Name is an optional name, which identifies the FORALL construct.

11.6.2 Array element ordering and physical and virtual memory

Fortran compilers will store arrays in memory according to the array element ordering scheme. Whilst the standard says nothing about how this is implemented it generally means in contiguous memory locations.

There will be a limit to the amount of physical memory available on any computer system. To enable problems that require more than the amount of physical memory available to be solved, most implementations will provide access to virtual memory, which in reality means access to a portion of a physical disk.

Access to virtual memory is commonly provided by a paging mechanism of some description. Paging is a technique whereby fixed-sized blocks of data are swapped between real memory and disk as required.

In order to minimise paging (and hence reduce execution time) array operations should be performed according to the array element order.

Some common page sizes are:

- Sun UltraSparc – 4Kb, 8Kb.
- DEC Alpha – 8Kb, 16Kb, 32Kb., 64Kb.
- Intel 80x86 – 4Kb.
- Intel Pentium PIII – 4Kb.

The Intel PIII also supports large pages (2Mb and 4Mb) — see the reference at the end of the chapter for more details.

11.7 Summary

We can now perform operations on whole arrays and partial arrays (array sections) without having to refer to individual elements. This shortens program development time and greatly clarifies the meaning of programs.

Array constructors can be used to assign values to rank 1 arrays within a program unit. The RESHAPE function allows us to assign values to a two or higher rank array when used in conjunction with an array constructor.

We have introduced the concept of a deferred-shape array. Arrays do not need to have their shape specified at compile time, only their rank. Their actual shape is deferred until runtime. We achieve this by the combined use of the ALLOCATABLE attribute on the variable declaration and the ALLOCATE statement, which makes Fortran a very flexible language for array manipulation.

11.8 Problems

1. Give the rank, bounds, extent and size of the following arrays:

```
REAL , DIMENSION(1:15) :: A
INTEGER , DIMENSION(1:3,0:4) :: B
REAL , DIMENSION(-2:2,0:1,1:4) :: C
INTEGER , DIMENSION(0:2,1:5) :: D
```

Which two of these arrays are conformable?

2. Use the SUM intrinsic function (see Appendix D) to calculate the total rainfall in the rainfall program example in Chapter 9.

3. Write a program to read in five rank 1 arrays, A, B, C, D, E and then store them as five columns in a rank 2 array TABLE.

4. Take the first part of Problem 2 in Chapter 10 and rewrite it using the SUM intrinsic function.

11.9 Bibliography

Bhandarkar D.P., *Alpha Implementation and Architecture: Complete Reference and Guide,* Digital Press.

Intel, *Intel Architecture Software Developer's Manual Volume 3: System Programming*

This is available as a PDF file from Intel. Try:

- http://developer.intel.com/design/PentiumIII/manuals/

12

Output of Results

"Why, sometimes I've believed as many as six impossible things before breakfast."

Lewis Carroll, *Through the Looking-Glass and What Alice Found There*

"All the persons in this book are real and none is fictitious even in part."

Flann O'Brien, *The Hard Life*

Aims

The aims here are to introduce the facilities for producing neat output and to show how to write results to a file, rather than to the terminal. In particular:

- The A, I, E, F, and X layout or edit descriptors.
- The OPEN, WRITE, and CLOSE statements.

12 Output of Results

When you have used PRINT * a few times it becomes apparent that it is not always as useful as it might be. The data are written out in a way which makes some sense, but may not be especially easy to read. Real numbers are written out with all their significant places, which is very often rather too many, and it is often difficult to line up the columns for data which are notionally tabular. It is possible to be much more precise in describing the way in which information is presented by the program. To do this, we use FORMAT statements. Through the use of the FORMAT we can:

- Specify how many columns a number should take up.
- Specify where a decimal point should lie.
- Specify where there should be white space.
- Specify titles.

The FORMAT statement has a label associated with it; through this label, the PRINT statement associates the data to be written with the form in which to write them.

12.1 Integers — I format or edit descriptor

Integer format is reasonably straightforward, and offers clues for formats used in describing other numbers. I3 is an integer taking three columns. The number is right justified, a bit of jargon meaning that it is written as far to the right as it will go, so that there are no trailing or following blanks. Consider the following example:

```
PROGRAM ch1201
INTEGER :: T
   PRINT *,' '
   PRINT *,' Twelve times table'
   PRINT *,' '
   DO T=1,12
      PRINT 100, T,T*12
      100 FORMAT(' ',I3,' *  12 = ',I3)
   END DO
END PROGRAM ch1201
```

The first statement of interest is

```
      PRINT 100, T,T*12
```

The 100 is a statement label. There must be a format statement with this label in the program. The variables to be written out are T and 12*T.

The second statement of interest is

```
100 FORMAT(' ',I3,' *  12 = ',I3)
```

Inside the brackets we have

''	Print out what occurs between the quote marks, in this case one space.
,	The comma separates items in the FORMAT statement.
I3	Print out the first variable in the PRINT statement right justified in three columns
,	Item separator.
'* 12 = '	Print out what occurs between the quote characters.
,	Item separator
I3	Print out the second variable (in this case an expression) right justified in three colums.

All of the output will appear on one line.

Now consider the following example:

```
program ch1202
implicit none
integer :: big=10
integer :: i
  do i=1,40
    print 100,i,big
    100 format(1x,i3,2x,i12)
    big=big*10
  end do
end program ch1202
```

The new feature in the format statement is the 1x and 2x edit descriptor. This is another way of getting white space into the output, and in this case one space and two spaces, respectively.

This program will loop and the variable big will overflow, i.e., go beyond the range of valid values for a 32-bit integer. Does the program crash or generate a run time error? This is the output from the NAG f95 compiler and the Intel Fortran 95 compiler.

```
 1              10
 2             100
 3            1000
 4           10000
 5          100000
 6         1000000
 7        10000000
 8       100000000
 9      1000000000
10      1410065408
11      1215752192
12      -727379968
13      1316134912
14       276447232
15     -1530494976
16      1874919424
17      1569325056
18     -1486618624
19     -1981284352
20      1661992960
21      -559939584
22     -1304428544
23      -159383552
24     -1593835520
25      1241513984
26      -469762048
27      -402653184
28       268435456
29     -1610612736
30      1073741824
31     -2147483648
32                0
33                0
34                0
35                0
36                0
37                0
38                0
39                0
40                0
```

Is there a compiler switch to trap this kind of error?

12.2 Reals — F format or edit descriptor

The F format can be seen as an extension of the integer format, but here we have to deal with the decimal point. The form of the F format specifies where the decimal point will occur, and how many digits follow it. Thus, F7.4 means:

- There is a total width of seven.
- There is a decimal point
- There are four digits after the decimal point.

This means that since the decimal point is also written out, there may be up to two digits before the decimal point. As in the case of the integer, any minus sign is part of the number, and would take up one column. Thus, the format F7.4 may be used for numbers in the range

–9.9999 to 99.9999

Let us look at the last example more closely. When a number is written out, it is rounded; that is to say, if we write out 99.99999 in an F7.4 format, the program will try to write out 100.0000! This is bad news, since we have not left enough room for all those digits before the decimal point. What happens? Asterisks will be printed. In the example above, a number out of range of the format's capabilities would be printed as:

```
*******
```

What would a format of F7.0 do? Again, seven columns have been set aside to accommodate the number and its decimal point, but this time no digits follow the point.

```
    99.
-21375.
```

are examples of numbers written in this format. With an F format, there is no way of getting rid of the decimal point.

The numbers making up the parts of the descriptors must all be positive integers. The definition of a real format is therefore F followed by two integer numbers, separated by a decimal point. The first integer must exceed the second, and the second must be greater than or equal to zero. The following are valid examples:

```
F4.0
F6.2
F12.2
F16.8
```

but these are *not* valid:

```
F4.4
F6.8
F-3.0
F6
F.2
```

The program in Section 12.2.1 illustrates the use of both I format and F format.

12.2.1 Metric and imperial conversion

```
program ch1203
implicit none
integer :: fluid
real :: litres
real :: pints
  do fluid=1,10
    litres = fluid / 1.75
    pints  = fluid * 1.75
    print 100 , pints,fluid,litres
    100 format(' ',F7.3,' ',I3,' ',F7.3)
  end do
end program ch1203
```

Pints will be printed out in F7.3 format, fluid will be printed out in I3 format and litres will be printed out in F7.3 format.

12.2.2 Overflow and underflow

Consider the following program:

```
program ch1204
implicit none
integer :: i
real     :: small = 1.0
real     :: big   = 1.0
  do i=1,50
    print 100,i,small,big
    100 format(' ',i3,' ',f7.3,' ',f7.3)
    small=small/10.0
    big=big*10.0
  end do
end program ch1204
```

In this program the variable small will underflow and big will overflow. The output from the Intel compiler is:

```
  1    1.000    1.000
  2    0.100   10.000
  3    0.010  100.000
  4    0.001  *******
  5    0.000  *******
  6    0.000  *******
  7    0.000  *******
  8    0.000  *******
  9    0.000  *******
 10    0.000  *******
 11    0.000  *******
 12    0.000  *******
 13    0.000  *******
 14    0.000  *******
 15    0.000  *******
 16    0.000  *******
 17    0.000  *******
 18    0.000  *******
 19    0.000  *******
 20    0.000  *******
 21    0.000  *******
 22    0.000  *******
 23    0.000  *******
 24    0.000  *******
 25    0.000  *******
 26    0.000  *******
 27    0.000  *******
 28    0.000  *******
 29    0.000  *******
 30    0.000  *******
 31    0.000  *******
 32    0.000  *******
 33    0.000  *******
 34    0.000  *******
 35    0.000  *******
 36    0.000  *******
 37    0.000  *******
 38    0.000  *******
 39    0.000  *******
 40    0.000   Infini
```

```
41    0.000   Infini
42    0.000   Infini
43    0.000   Infini
44    0.000   Infini
45    0.000   Infini
46    0.000   Infini
47    0.000   Infini
48    0.000   Infini
49    0.000   Infini
50    0.000   Infini
```

When the number is too small for the format, the printout is what you would probably expect. When the number is too large, you get asterisks. When the number actually overflows the Intel compiler tells you that the number is too big and has overflowed. However the program ran to completion and did not generate a run time error.

12.3 Reals — E format or edit descriptor

The exponential or scientific notation is useful in cases where we need to provide a format which may encompass a wide range of values. If likely results lie in a very wide range, we can ensure that the most significant part is given. It is possible to give a very large F format, but alternatively, the E format may be used. This takes a form such as

```
E10.4
```

which looks something like the F, and may be interpreted in a similar way. The 10 gives the total *width* of the number to be printed out, that is, the number of columns it will take. The number after the decimal point indicates the number of positions to be written after the decimal point. Since all exponent format numbers are written so that the number is between 0.1 and 0.9999..., with the exponent taking care of scale shifts, this implies that the first four significant digits are to be printed out.

Taking a concrete example, 1000 may be written as 10**3, or as 0.1 * 10**4. This gives us the two parts: 0.1 gives the significant digits (in this case only one significant digit), while the 10**4 gives the exponent, namely 4 or +4. In a form that looks more like Fortran, this would be written .1E+04, where the E+04 means 10**4.

There is a minimum *size* for an exponential format. Because of all the extra bits and pieces it requires:

- The decimal point.

- The sign of the entire number.
- The sign of the exponent.
- The magnitude of the exponent.
- The E.

The width of the number less the number of significant places should not be less than 6. In the example given above, E10.4 meets this requirement. When the exponent is in the range 0 to 99, the E will be printed as part of the number; when the exponent is greater, the E is dropped, and its place is taken by a larger value; however, the sign of the exponent is always given, whether it is positive or negative. The sign of the whole number will usually only be given when it is negative. This means that if the numbers are always positive, the *rule of six* given above can be modified to a *rule of five*. It is safer to allow six places over, since, if the format is insufficient, all you will get are asterisks.

The most common mistake with an E format is to make the edit descriptor too small, so that there is insufficient room for all the *padding* to be printed. Formats like E8.4 just don't work (on output anyway). The following four are valid E formats on output:

```
E9.3
E11.2
E18.7
E10.4
```

but the next five would not be acceptable as output formats, for a variety of reasons:

```
E11.7
E6.3
E4.0
E10
E7.3
```

12.3.1 Simple E format example

This is the same as ch1204 except that we have replaced the F formatting with E formatting:

```
program ch1205
implicit none
integer :: i
real    :: small = 1.0
real    :: big   = 1.0
```

```
   do i=1,50
     print 100,i,small,big
     100 format(' ',i3,' ',e10.4,' ',e10.4)
     small=small/10.0
     big=big*10.0
   end do
end program ch1205
```

We now have three ways to print out floating point numbers and each has its use. The PRINT * is very useful when developing programs.

12.4 Spaces

You have seen two ways of generating spaces on output. The first is to use ' characters to enclose blanks in the format statement. The second is to use the X edit descriptor. Consider the following.

```
PRINT 100, ALPHA,BETA
100 FORMAT(1X,F10.4,10X,F10.3)
```

The 10X is read rather like any of the other format elements — logically it should have been X10, to correspond to I10 or F10.4, but that would be allowing intuition to run away with you. Clearly the X3J3 committee felt it important that Fortran should have inconsistencies, just like a natural language.

Remember that these blanks are in addition to any generated as a result of the leading blanks on numbers (if any are present). If you wish to leave a single space, you must still precede the X by a number (in this case, 1); simply writing X is illegal. The general form is therefore a positive integer followed by X.

12.5 Characters — A format or edit descriptor

This is perhaps the simplest output of all. Since you will already have declared the length of a character variable in your declarations,

```
CHARACTER (10) :: B
```

when you come to write out B, the length is known — thus you need only specify that a character string is to be output:

```
PRINT 100,B
100 FORMAT(1X,A)
```

If you feel you need a little extra control, you can append an integer value to the A, like A10 (A9 or A1), and so on. If you do this, only the first 10 (9 or 1) char-

acters are written out; the remainder are ignored. Do note that 10A1 and A10 are not the same thing. 10A1 would be used to print out the first character of ten character variables, while A10 would write out the first 10 characters of a single character variable. The general form is therefore just A, but if more control is required, this may be followed by a positive integer.

The following program is a simple rewrite of a program from Chapter 7.

```
PROGRAM ch1206
!
! This program reads in and prints out
! your first name
!
IMPLICIT NONE
CHARACTER (20) :: First_name
!
   PRINT *,' Type in your first name.'
   PRINT *,' up to 20 characters'
   READ *,First_Name
   PRINT 100,First_Name
   100 FORMAT(1x,A)
!
END PROGRAM ch1206
```

12.5.1 Headings

A simple heading is given in the program below:

```
program ch1207
implicit none
integer :: fluid
real :: litres
real :: pints
   PRINT *,' Pints        Litres'
   do fluid=1,10
     litres = fluid / 1.75
     pints  = fluid * 1.75
     print 100 , pints,fluid,litres
     100 format(' ',f7.3,' ',i3,' ',f7.3)
   end do
end program ch1207
```

12.6 Mixed type output in a FORMAT statement

The following example shows how to mix and match character, integer and real output in one FORMAT statement:

```
PROGRAM ch1208
IMPLICIT NONE
CHARACTER (LEN=15) :: Firstname
INTEGER :: age
REAL :: weight
CHARACTER (LEN=1) :: sex
   PRINT *,' Type in your first name '
   READ *,Firstname
   PRINT *,' type in your age in years'
   READ *,age
   PRINT *,' type in your weight in kilos'
   READ *,weight
   PRINT *,' type in your sex (f/m)'
   READ *,sex
   PRINT *,' your personal details are'
   PRINT *
   PRINT 100
   100 FORMAT(4x,'first name', 4x , 'age' , 1x , &
       'weight' , 2x , 'sex')
   PRINT 200 , firstname, age , weight , sex
   200 FORMAT(1x , a , 2x , i3 , 2x , f5.2 , 2x, a)
END PROGRAM ch1208
```

Take care to match up the variables with the appropriate edit descriptors. You also need to count the number of characters and spaces when lining up the heading.

12.7 Common mistakes

It must be stressed that an integer can only be printed out with an I format, and a real with an F (or E) format. You cannot use integer variables or expressions with F or E edit descriptors or real variables and expressions with I edit descriptors. If you do, unpredictable results will follow. There are (at least) two other sorts of errors you might make in writing out a value. You might try to write out something which has never actually been assigned a value; this is termed an indefinite value. You might find that the letter I is written out. In passing, note that many loaders and link editors will preset all values to zero — i.e., unset (indefinite) values are actually set to zero. On better systems there is generally some way of turning this facility off, so that undefined is really indefinite. More often than not, indefinite values are the result of mistyping rather than of never setting values. It is not un-

common to type O for 0, or 1 for either I or l. The other likely error is to try to print out a value greater than the machine can calculate — *out of range* values. Some machines will print out such values as R, but some will actually print out something which looks right, and such *overflow* and *underflow* conditions can go unnoticed. Be wary.

12.8 OPEN (and CLOSE)

One of the particularly powerful features of Fortran is the way it allows you to manipulate files. Up to now, most of the discussion has centred on reading from and writing to the terminal. It is also possible to read and write to one or more files. This is achieved using the OPEN, WRITE, READ and CLOSE statements. In a later chapter we will consider *reading* from files but here we will concentrate on *writing*.

12.8.1 The OPEN statement

This statement sets up a file for either reading or writing. A typical form is

```
OPEN (UNIT=1,FILE='DATA')
```

The file will be known to the operating system as DATA (or will have DATA as the first part of its name), and can be written to by using the UNIT number. This statement should come *before* you first read from or write to the file DATA.

It is not possible to write to the file DATA directly; it must be referenced through its unit number. Within the Fortran program you write to this file using a statement such as

```
WRITE(UNIT=1,FMT=100) XVAL,YVAL
```

or

```
WRITE(1,100) XVAL,YVAL
```

These two statements are equivalent. Besides opening a file, we really ought to CLOSE it when we have finished writing to it:

```
CLOSE(UNIT=1)
```

In fact, on many systems it is not obligatory to OPEN and CLOSE all your files. Almost certainly, the terminal will not require this, since INPUT and OUTPUT units will be there by default. At the end of the job, the system will CLOSE all your files. Nevertheless, explicit OPEN and CLOSE cannot hurt, and the added clarity generally assists in understanding the program.

The following program contains all of the above statements:

```
program ch1209
implicit none
integer :: fluid
real :: litres
real :: pints
   open (unit=1,file='ch1209.txt')
   write(unit=1,fmt=200)
   200 format(' Pints        Litres')
   do fluid=1,10
      litres = fluid / 1.75
      pints  = fluid * 1.75
      write(unit=1,fmt=100) , pints,fluid,litres
      100 format(' ',f7.3,' ',i3,' ',f7.3)
   end do
   close(1)
end program ch1209
```

12.8.2 Writing

PRINT is always directed to the file OUTPUT; in the case of interactive working, this is the terminal. This is not a very flexible arrangement. WRITE allows us to direct output to any file, including *OUTPUT*. The basic form of the WRITE is

```
WRITE(6,100) X,Y,Z
```

or

```
WRITE(UNIT=6,FMT=100) X,Y,Z
```

The latter form is more explicit, but the former is probably the one most widely used. We have an example here of the use of positionally dependent parameters in the first case and equated keywords in the second. With the exceptions of the PRINT statement and the READ * form of the READ, all of the input/output statements allow the unit number and the format labels to be specified either by an equated keyword (or specifier) or in a positionally dependent form. If you use the explicit UNIT= and FMT= it does not matter what order the elements are placed in, but if you omit these keywords, the unit number must come first, followed by the format label.

UNIT=6 means that the output will be written to the file given the unit number 6. In the next chapter we will cover the way in which you may associate file names and unit numbers, but, for the moment, we will assume that the default is being used. The name of the file, as defined by the system, will depend on the particular system you use; a likely name is something like DATA06, TAPE6, or FILE0006. One *easy* way to find out (apart from asking someone) is to create such a file from

a program and then look at the names of your files after the program has finished. A great many of computing's minor complexities can be clarified by simple experimentation.

FMT=100 simply gives the label of the format to be used.

The overworked asterisk may be used, either for the unit or for the format:

UNIT=* will write to OUTPUT (the terminal)

FMT=* will produce output controlled by the list of variables, often called *list directed output.*

The following three statements are therefore equivalent:

```
WRITE(UNIT=*,FMT=*) X,Y,Z
WRITE(*,*) X,Y,Z
PRINT*,X,Y,Z
```

There are other controls possible on the WRITE, which will be elaborated later.

12.9 Repetition

Often we need to print more than one number on a line and want to use the same layout descriptor. Consider the following:

```
PRINT 100,A,B,C,D
```

If each number can be written with the same layout descriptor, we can abbreviate the FORMAT statement to take account of the pattern:

```
100 FORMAT(1X,4F8.2)
```

is equivalent to

```
100 FORMAT(1X,F8.2,F8.2,F8.2,F8.2)
```

as you might anticipate. If the pattern is more complex, we can extend this approach:

```
PRINT 100,I,A,J,B,K,C
100 FORMAT(1X,3(I3,F8.2))
```

Bracketing the description ensures that we repeat the whole entity:

```
100 FORMAT(1X,3(I3,F8.2))
```

is equivalent to

```
100 FORMAT(1X,I3,F8.2, I3,F8.2, I3,F8.2)
```

Repetition with brackets can be rather more complex. In order to give some overview of formatted Fortran output, it is helpful to delve a little into the history of the language. Many of the attributes of Fortran can be traced back to the days of single-user mainframes (with often a fraction of the power of many contemporary microcomputers and workstations). These would generally take input from punched cards (the traditional 80-column Hollerith card), and would generate output on a line printer. In this sort of environment, the individual punched card had a significance which lines in a file do not have today. Each card could be seen as a single entity — a physical record unit. The *record* was seen as an element of a subdivision within a file. Even then, there was some confusion between the notion of physical records and files split into logically distinct subunits, since these subunits might also be termed records. The present Fortran standard merely says that a record *does not necessarily correspond to a physical entity*, although *a punched card is usually considered to be a record.* This leaves us sitting at our terminals in a bemused state, especially since we may have no idea what a punched card looks like (an ideal state of affairs!).

It is important to have some notion of a record, since most of the formal definitions dealing with output (and input) are couched in terms of records. Every time an input or output statement is executed your nominal position in the file changes. If we think in terms of individual records (which may be cards), the notions of *current, preceding* and *next* record seem fairly straightforward. The current record is simply the one we have just read or written, and the other definitions follow naturally.

The situation becomes less clear when we realise that a single output statement may generate many lines of output:

```
WRITE(UNIT=6,FMT=101)   A,B,C
101  FORMAT(1X,F10.4)
```

writes out three separate lines. Looking at the output alone, there is no way to distinguish this from the output generated by

```
WRITE(UNIT=6,FMT=101)   A
WRITE(UNIT=6,FMT=101)   B
WRITE(UNIT=6,FMT=101)   C
101  FORMAT(1X,F10.4)
```

In the latter case we would probably be happy to consider each line a *record,* although in the previous example we might swither between considering all three lines (generated by a single statement) a single record or three records. Consider the first of these two examples more closely; each time the format is exhausted — that is to say, each time we run out of format description, we start again on a new

line (a new record). A new record is begun as each F10.4 is begun. The correct interpretation is therefore that three records have been written.

The same sort of thing happens in more complex FORMAT statements:

```
WRITE(UNIT=6,FMT=105) X,I,Y
105 FORMAT(1X,F8.4,I3,(F8.4))
```

would write out a single record containing a real, an integer and a real. Using the same format statement with WRITE (UNIT=6, FMT=105) X,I,Y,Z would write out two records. The first containing the values of X, I and Y and the second containing only Z. If there were still more values

```
WRITE(UNIT=6,FMT=105) X,I,Y,Z,A
```

would print out three records. The group in brackets — the (F8.4) — is repeated until we run out of items.

12.10 Some more examples

Since it is the last open bracket which determines the position at which the format is repeated, simply writing

```
WRITE(UNIT=6,FMT=100)   A,I,B,C,J
100 FORMAT(1X,F8.4,I3,F8.2)
```

would imply that A, I and B would be written on one line then, returning to the last open brackets (in this case the only open brackets), a new record (or line) is begun to write out C and J. A statement like

```
100 FORMAT(1X,(F8.4),I3,F8.2)
```

would return to the (F8.4) group, and then continue to the I3 and F8.2 before repeating again (if necessary). The same thing happens if the (F8.4) had no brackets around it. On the other hand

```
100 FORMAT(1X,(F8.4),I3,(F8.2))
```

contains superfluous brackets around the F8.4, since the repeat statement will never return to that group. Are you confused yet? This all seems very esoteric, and really, we have only hinted at the complexity which is possible. It is seldom that you have to create complex FORMAT statements, and clarity is far more important than brevity.

When patterned or repeated output is used, we may want to stop when there are no more numbers to write out. Take the following example:

```
   WRITE(UNIT=1,FMT=100) A,B,C,D
   100 FORMAT(1X,4(F6.1,','))
```

This will give output which looks like

```
 37.4,   29.4,   14.2,   -9.1,
```

The last comma should not be there. We can suppress these unwanted elements by using the colon:

```
   100 FORMAT(1X,4(F6.1:','))
```

which would then give us

```
 37.4,   29.4,   14.2,   -9.1
```

Since we run out of data at the fourth item, D, the output following is not written out. It is a small point, but it does look a lot tidier. There are other ways of achieving the same thing.

This helps to illustrate another point, namely that you may have formats which are more extensive than the lists which reference them:

```
   WRITE(UNIT=1,FMT=100) A,B,C
   WRITE(UNIT=1,FMT=100) X,Y
   100 FORMAT(1X,6F8.2)
```

Both WRITE statements use the format provided, although they write out different numbers of data, and neither uses up the whole format.

12.11 Implied DO loops and array sections for array output

The following program shows how to use both implied DO loops and array sections to output an array in a neat fashion:

```
program ch1210
implicit none
integer , parameter :: nrow=5
integer , parameter :: ncol=6
real , dimension(1:nrow*ncol)    :: results = &
                 (/50 , 47 , 28 , 89 , 30 , 46 , &
                   37 , 67 , 34 , 65 , 68 , 98 , &
                   25 , 45 , 26 , 48 , 10 , 36 , &
                   89 , 56 , 33 , 45 , 30 , 65 , &
                   68 , 78 , 38 , 76 , 98 , 65/)
```

```
REAL , DIMENSION(1:nrow,1:ncol) :: Exam_Results     =
0.0
real , dimension(1:nrow)          :: People_average   =
0.0
real , dimension(1:ncol)          :: Subject_Average =
0.0
integer :: r,c
  exam_results = &
  reshape(results,(/nrow,ncol/),(/0.0,0.0/),(/2,1/))
  Exam_Results(1:nrow,3) = 2.5 * Exam_Results(1:nrow,3)
  subject_average = sum(exam_results,dim=1)
  people_average  = sum(exam_results,dim=2)
  people_average  = people_average  / ncol
  subject_average = subject_average / nrow
  do r=1,nrow
    print 100 , (exam_results(r,c),c=1,ncol) ,&
      people_average(r)
    100 format(1x,6(1x,f5.1),'  = ',f6.2)
  end do
  print *,'  ====  ====  ====  ====  ====  ====  ====='
  print 110, subject_average(1:ncol)
  110 format(1x,6(1x,f5.1))
end program ch1210
```

The print 100 uses an implied DO loop and the print 110 uses an array section.

Take care when using whole arrays. Consider the following program:

```
PROGRAM ch1211
REAL , DIMENSION(10,10) :: Y
INTEGER :: NROWS=6
INTEGER :: NCOLS=7
INTEGER :: I,J
INTEGER :: K=0

  DO I=1,NROWS
    DO J=1,NCOLS
      K=K+1
      Y(I,J)=K
    END DO
  END DO

  WRITE(UNIT=*,FMT=100)Y
```

```
  100 FORMAT(1X,10F10.4)

END PROGRAM ch1211
```

There are several points to note with this example. Firstly, this is a whole array reference, and so the entire contents of the array will be written; there is no scope for fine control. Secondly, the order in which the array elements are written is according to Fortran's array element ordering, i.e., the first subscript varying 1 to 10 (the array bound), with the second subscript as 1, then 1 to 10 with the second subscript as 2 and so on; the sequence is

```
Y(1,1)   Y(2,1)   Y(3,1)       Y(10,1)
Y(1,2)   Y(2,2)   Y(3,2)       Y(10,2)
   .
   .
Y(1,10)  Y(2,10)               Y(10,10)
```

Thirdly we have defined values for part of the array. This program behaves differently with the following compilers:

- Sun Fortran 90.
- NagWare F95.
- Compaq F95.

If you have access to more than one compiler then try out this example.

12.12 Formatting for a line printer

There is one extension to format specifications which is relevant to line printers. Fortran defines four special characters which have an effect on standard line printers when they occur in the first character position of a line. This means that a lineprinter which is not under your immediate control can be used to produce neat output by sending a file to be printed on it. This has a variety of names including, *spooling*, *queueing* and *routing* depending on the system. You should check with your local system for the exact mechanism to achieve this.

The special characters are +, 0, 1 and blank. To be used, they must be the first character of the output in each line — as if they were to be printed in column 1. In fact, a standard line printer never prints a character that occurs in column 1 at all.

Whenever a WRITE statement is begun, the printer *advances* to a new record; i.e., a new line is begun before any data are transferred. If the first character is a *special character,* then this will be interpreted by the line printer. If the first character

to be printed is a blank, the printer continues printing on that line. The first character is also known as the *carriage control character.*

The blank is a *do nothing special* control. It signifies that the line is to be printed as it is.

The zero indicates that you wish to leave an extra line; this is often useful in spacing out results to make the output more readable.

The 1 makes the output skip down to the top of the next page. This is clearly useful for separating logically distinct chunks of output. If you obtain a line printer listing of your compiled program, each segment will start at the top of a new page.

The plus is a *no advance* or *overprint* character. It suppresses the effect of the line advance which a WRITE generates. No new line is begun and the previous line is overprinted with the new. Overprinting can be useful especially when you wish to print out grey scale maps but its use is rather restricted. In particular, it can be a dangerous control character. If you have a format starting with a plus in a loop, you can make the printer overprint again and again and again . . . and again and again, until it has hammered itself into a pulp. This is not a good idea.

Similarly, accidental use of the 1 as a control character in a loop will give you lots of blank pages. It is just a bit embarrassing to be presented with a 6 inch stack of paper which is (almost) blank, because you had a 1 repeatedly in column 1.

12.12.1 Mechanics of carriage control

The following are all quite reasonable ways of generating the blank in column 1:

```
WRITE(UNIT=6,FMT=100)A
100 FORMAT(' ',F10.4)
```

or

```
WRITE(UNIT=6,FMT=100)A
100 FORMAT(1X,F10.4)
```

or

```
WRITE(UNIT=6,FMT=100)A
100 FORMAT(' THE ANSWER IS ',F10.4)
```

Note, however, that

```
WRITE(UNIT=6,FMT=100)A
100 FORMAT(F8.4)
```

could result in problems. If A contained the value 100.2934, the result on a line printer would be

```
00.2934
```

printed at the top of a new page. The 1 is taken as carriage control, and the rest of the line then printed.

Accidentally printing zeros in column 1 is a little more difficult, but

```
WRITE(UNIT=6,FMT=100)I
100 FORMAT(I1)
```

might just do it. Don't.

Remember that this only applies to line printer output, and not to the terminal. Since Fortran only defines four characters as carriage control, you will find that anything else in column 1 will give unpredictable results. On some systems, a fair number of alternatives may be defined by the installation, and they may do something useful. On other systems, they may do something, but they may also fail to print the rest of the line. This can be very perplexing. Beware.

12.12.2 Generating a new line on both line printers and terminals

There are several ways of generating new lines, other than with a 0 in column 1 of your line printer output. A more general approach, which works on both terminals and line printers, is through the oblique or slash, /. Each time this is encountered in a FORMAT statement, a new line is begun.

```
PRINT 101,A,B
101 FORMAT(1X,F10.4/1X,F10.4)
```

would give output like

```
 100.2317
-4.0021
```

This is the same as (F10.4) would have given, but clearly it opens up lots of possibilities for formatting output more tidily:

```
PRINT 102,NVAL,XMAX,XMIN
102 FORMAT(' NUMBER OF VALUES READ IN WAS: ',I10/ &
          ' MAXIMUM VALUE IS: ',F10.4/            &
          ' MINIMUM VALUE IS: ',F10.4)
```

may be easier to read than using only one line, and it is certainly more compact to write than using three separate print statements. It is not necessary to separate / by commas, although if you do nothing catastrophic will happen.

You may also begin a format description with a /, in order to generate an extra line or even generate lots of lines with lots of slashes; e.g.,

```
WRITE(UNIT=6,FMT=103)A,B
103 FORMAT(//1X,F10.4,4(/),1X,F10.4)
```

will leave two lines before printing A, and then will generate four new lines before writing B (i.e., there will be three lines between A and B — the fourth new line will contain B). While a slash by itself, or with another slash, does not have to be separated by commas from other groups, a more complex grouping, 4(/), does have to have commas and brackets to delimit it.

12.13 Timing of writing formatted files

The following example looks at the amount of time spent in different sections of a program with the main emphasis on formatted output:

```
program ch1212
implicit none
integer , parameter :: n=1000000
integer , dimension(1:n) :: x
real    , dimension(1:n) :: y
integer :: i
real :: t,t1,t2,t3,t4,t5
character*10 :: comment
  open(unit=10,file='ch1212.txt')
  call cpu_time(t)
  t1=t
  comment=' Intial '
  print 100,comment,t1
  do i=1,n
    x(i)=i
  end do
  call cpu_time(t)
  t2=t-t1
  comment = ' Integer '
  print 100,comment,t2
  y=real(x)
  call cpu_time(t)
  t3=t-t1-t2
```

```
   comment = ' real '
   print 100,comment,t2
   do i=1,n
     write(10,200) x(i)
     200 format(1x,i10)
   end do
   call cpu_time(t)
   t4=t-t1-t2-t3
   comment = ' i write '
   print 100,comment,t4
   do i=1,n
     write(10,300) y(i)
     300 format(1x,f10.0)
   end do
   call cpu_time(t)
   t5=t-t1-t2-t3-t4
   comment = ' r write '
   print 100,comment,t5
   100 format(1x,a,2x,f7.3)
end program ch1212
```

There is a call to the built-in intrinsic cpu_time to obtain timing information. Timing details for a number of compilers follow:

	Intel	**Nag**	**Salford**
Intial	0.063	0.046	0.094
Integer	0.031	0.031	0.016
real	0.031	0.031	0.016
i write	10.109	16.968	2.453
r write	12.281	101.860	3.453

Formatted output takes up a lot of time, as we are converting from an internal binary representation to an external decimal form.

12.14 Timing of writing unformatted files

The following program is a variant of the above but now the output is in unformatted or binary form:

```
program ch1213
implicit none
integer , parameter :: n=1000000
integer , dimension(1:n) :: x
real    , dimension(1:n) :: y
```

```
integer :: i
real :: t,t1,t2,t3,t4,t5
character*10 :: comment
  open(unit=10,file='ch1213.txt',form='unformatted')
  call cpu_time(t)
  t1=t
  comment=' Intial '
  print 100,comment,t1
  do i=1,n
    x(i)=i
  end do
  call cpu_time(t)
  t2=t-t1
  comment = ' Integer '
  print 100,comment,t2
  y=real(x)
  call cpu_time(t)
  t3=t-t1-t2
  comment = ' real '
  print 100,comment,t2
  write(10) x
  call cpu_time(t)
  t4=t-t1-t2-t3
  comment = ' i write '
  print 100,comment,t4
  write(10) y
  call cpu_time(t)
  t5=t-t1-t2-t3-t4
  comment = ' r write '
  print 100,comment,t5
  100 format(1x,a,2x,f7.3)
end program ch1213
```

Timing details for a number of compilers follows:

	Intel	**Nag**	**Salford**
Intial	0.063	0.062	0.172
Integer	0.031	0.030	0.031
real	0.031	0.030	0.031
i write	0.031	0.064	0.063
r write	0.031	0.062	0.063

Unformatted is very efficient in terms of time. It also has the benefit for real or floating point numbers of no information loss.

In Chapter 13 we will look at timing information reading in formatted and unformatted files.

12.15 Summary

You have been introduced in this chapter to the use of format or layout descriptors which will give you greater control over output.

The main features are:

- The I format for integer variables.
- The E and F formats for real numbers.
- The A format for characters.
- The X, which allows insertion of spaces.

Output can be directed to files as well as to the terminal through the WRITE statement.

The WRITE, together with the OPEN and CLOSE statements, also introduces the class of Fortran statements which use equated keywords, as well as positionally dependent parameters.

The FORMAT statement and its associated layout or edit descriptor are powerful and allow repetition of patterns of output (both explicitly and implicitly).

When output is to be directed to a line printer, the following four characters:

- +
- 0
- 1
- (blank)

allow reasonable control over the layout. Care must to be taken with these characters, since it is possible to decimate forests with little effort.

12.16 Problems

1. Rewrite the temperature conversion program which was Problem 8 in Chapter 10 to actually produce the output shown.

2. Write a litres and pints conversion program to produce a similar kind of output to problem one above. Start at 0 and make the central column go up to 50. One pint is 0.568 litres.

3. Information on car fuel consumption is usually given in miles per gallon in Britain and the United States and in litres per 100 kilometres in Europe. Just to add an extra problem US gallons are 0.8 imperial gallons.

Prepare a table which allows conversion from either US or imperial fuel consumption figures to the metric equivalent. Use the PARAMETER statement where appropriate:

1 imperial gallon = 4.54596 litres
1 mile = 1.60934 kilometres

4. The two most commonly used operating systems for Fortran programming are UNIX and DOS. It is possible to use the operating system file redirection symbols < and > to read from a file and write to a file, respectively. Rerun the program in problem 1 to write to a file. Examine the file using an editor.

5. Modify any of the above to write to a file rather than the terminal. What changes are required to produce a general output which will be suitable for both the terminal and a line printer? Is this degree of generality worthwhile?

6. To demonstrate your familiarity with formats, reformat problems 1, 2 or 3 to use E formats, rather than F (or vice versa).

7. Modify the temperature conversion program to produce output suitable for a line printer. Use the local operating system commands to send the file to be printed.

8. Repeat for the litres and pints program.

9. What features of Fortran reveal its evolution from punched card input?

10. Try to create a real number greater than the maximum possible on your computer — write it out. Try to repeat this for an integer. You may have to exercise some ingenuity.

11. Check what a number too large for the output format will be printed as on your local system — is it all asterisks?

12. Write a program which stores litres and corresponding pints in arrays. You should now be able to control the output of the table (excluding headings — although this could be done too) in a single WRITE or PRINT statement. If you don't like litres and pints, try some other conversion (£ sterling to US dollars, leagues to fathoms, Scots miles to Betelgeusian pfnings). The principle remains the same.

13. Fortran is an old programming language and the text formatting functionality discussed in this chapter assumes very dumb printing devices.

The primary assumption is that we are dealing with so-called monospace fonts, i.e., that digits, alphabetic characters, punctuation, etc., all have the same width.

If you are using a PC try using:

- Notepad

and

- Word

to open your programs and some of the files created in this chapter. What happens to the layout?

If you are using Notepad look at the *Word wrap* and *set Font* options under the *edit* menu.

What fonts are available? What happens to the layout when you choose another font?

If you are using Word what fonts are available? What happens when you make changes to your file and exit Word? Is it sensible to save a Fortran source file as a Word document?

13

Reading in Data

"Winnie-the-Pooh read the two notices very carefully,
first from left to right, and afterwards,
in case he had missed some of it, from right to left."

A A Milne, *Winnie-the-Pooh*

"For Madmen Only"

Hermann Hesse, *Steppenwolf*

Aims

The aims of this chapter are to introduce some of the ideas involved in reading data into a program. In particular, using the following:

- Reading from fixed fields.
- Integers, reals and characters.
- Blanks — nulls or zeros?
- READ — extensions.
    - error handling on input.
- OPEN — associating unit numbers and file names.
    - CLOSE
    - REWIND
    - BACKSPACE

13 Reading in Data

13.1 Reading from the terminal or keyboard versus reading from files

It is unlikely that you would use fixed formats when reading numeric input from the terminal or keyboard; they are more likely to be used when reading data from a file. However the examples that follow do it. We look at reading from files later in this chapter.

13.2 Fixed fields on input

All the formats described earlier are available, and again they are limited to particular types. Integers may only be input by the I format, reals with F and E, and character (alphanumeric) with A.

13.2.1 Integers and the I format

Integers are read in with the I edit descriptor. Whereas, on output, integers appear right justified, on input they may appear anywhere in the field you have delimited. Blanks (by default) are considered not to exist for the purpose of the value read, although they do contribute to the field width. Apart from the digits 0 to 9, the only other characters which may appear in an integer field are – and +.

Consider the following 12 times table:

```
 1 *  12 =  12
 2 *  12 =  24
 3 *  12 =  36
 4 *  12 =  48
 5 *  12 =  60
 6 *  12 =  72
 7 *  12 =  84
 8 *  12 =  96
 9 *  12 = 108
10 *  12 = 120
11 *  12 = 132
12 *  12 = 144
```

The following is a program to read the first and last columns of integer data:

```
program ch1301
implicit none
integer , parameter :: n=12
integer :: i
```

```
integer , dimension(1:n) :: x
integer , dimension(1:n) :: y
  do i=1,n
    read  100,x(i),y(i)
    100 format(2x,i2,9x,i3)
    print 200,x(i),y(i)
    200 format(1x,i3,2x,i3)
  end do
end program ch1301
```

The

```
    read  100,x(i),y(i)
```

will try reading values into x(i) and y(i) using format statement

```
    100 format(2x,i2,9x,i3)
```

which will skip the first two characters on the line or record, read the first value from the next two columns, skip the next nine characters and read the last value from the next three characters.

We recommend that when working with formatted files you to use a text editor that displays the column and line details

Notepad under Windows has a status bar option under the View menu. Gvim under Windows has line and column information available. Under Redhat, vim and gedit both display line and column information. User SuSe, kedit and vim display line and column information. There should be an editor available on your system that has this option.

13.2.2 Reals and the F format

Real numbers may be input using a variety of formats and we will look at the F fomat in this example. Consider the following BMI data:

```
1.85  85
1.80  76
1.85  85
1.70  90
1.75  69
1.67  83
1.55  64
1.63  57
1.79  65
1.78  76
```

The following program will read in the data:

```
program ch1302
implicit none
integer , parameter :: n=10
real , dimension(1:n) :: h
real , dimension(1:n) :: w
real , dimension(1:n) :: bmi
integer :: i
  do i=1,n
    read 100, h(i),w(i)
    100 format(f4.2,2x,f3.0)
  end do
  bmi=w/(h*h)
  do i=1,n
    print 200,bmi(i)
    200 format(2x,f5.0)
  end do
end program ch1302
```

To read in the heights we need a total width of four columns with two after the decimal point. We then skip two spaces and read in the weights. The data in the file do not have a decimal point!

13.2.3 Reals and the E Format

An exponential format number (which may be read in F or E formats) can take a number of different forms. The most obvious is the explicit form

```
-1.2E-4
```

where all the components of the value are present — the significant digits to the left of the E, the E itself, and the exponent to the right. We can drop (almost) any two of these three components, so:

```
-1.2
-1.2E
-1.2-4
-4
```

are all valid values. Only the first two are interpreted as the same numerical value, and just giving the exponent part would be interpreted by the format as giving only the significant digits. If the exponent is to be given, there must be some significant digits as well. It is not even enough to give the E and assume that the program will interpret this as 10 to the power *exponent*.

```
E-4
```

is not an acceptable exponential format value, although

```
1E-4
```

would be.

There are opportunities for confusion with E formats.

```
READ(UNIT=*,FMT=102) X,Y
102 FORMAT(2E10.3)
```

with:

```
10.23 -2
```

would be interpreted as X taking the value 10.23E-2 and Y taking the value 0.0, while with

```
102 FORMAT(2F8.3)
```

X would be 10.23, and Y would be –2.0.

Although the decimal point may also be dropped, this might generate confusion as well. While

```
4E3
45
45E-4
45-4
```

are all valid forms, if an E format is used, a special conversion takes place. A format like E10.8, when used with integral significant digits (no decimal point), uses the 8 as a *negative* power of 10 scaling e.g.'

```
3267E05
```

converts to

```
3267*10**8*10**5
```

or

```
3267*10**3
```

or

3.267

Therefore, the interpretation of, say, 136, read in E format, would depend on the format used:

Value	Format		Interpretation
136	E10.0		136.0
136	E10.4		136.0*10**–4
		or	0.0136
136	E10.10		136.0*10**–10
		or	0.0000000136
136.	Any above		136.0

One implication of all this is that the format you use to input a variable may not be suitable to output that same variable. So given the data:

```
136
136
136
136
136.
136.
136.
136.
```

and the program

```
program ch1303
implicit none
real     :: x
  read 100,x
  100 format(e10.0)
  print *,x
  read 200,x
  200 format(e10.4)
  print *,x
  read 300,x
  300 format(e10.10)
  print *,x
  read *,x
```

```
   print *,x
   read 100,x
   print *,x
   read 200,x
   print *,x
   read 300,x
   print *,x
   read *,x
   print *,x
end program ch1303
```

We get the following output when the program is compiled with the Intel compiler:

```
    136.0000
  1.3600000E-02
  1.3600000E-08
    136.0000
    136.0000
    136.0000
    136.0000
    136.0000
```

Other compilers may give slightly different formatting of the output.

13.3 Blanks, nulls and zeros

You can control how Fortran treats blanks in input through two special format instructions, BN and BZ. BN is a shorthand form of *blanks become null,* that is, a blank is treated as if it were not there at all. BZ is therefore *blanks become zeros.*

As we have already seen, 1 4 (i.e., the two digits separated by a blank) read in I3 format would be read as 14; similarly, 14 (one-four-blank) is also 14 when the BN format is in operation. All of the blanks are ignored for the purposes of interpreting the number. They help to create the width of the number, but otherwise contribute nothing. This is the default, which will be in operation unless you specify otherwise.

The BZ descriptor turns blanks into zeros. Thus, 1 4 (one-blank-four) read in I3 format is 104, and 14 (one-four-blank) is 140.

There is one place where we must be very careful with the use of the BZ format — when using exponent format input. Consider

```
5.321E+02
```

read in (BZ,E10.3) format. We have specified a field which is ten characters wide; therefore the blank in column 10, which follows the E+02, is read as a zero, making this E+020. This is probably not what was required.

13.4 Characters

When characters are read in, it is sufficient to use the A format, with no explicit mention of the size of the character string, since this size (or length) is determined in the program by the CHARACTER declaration. This implies that any *extra* characters would not be read in. You may however read in less:

```
CHARACTER (10) :: LIST
    .
    .
   READ(UNIT=5,FMT=100)LIST
   100 FORMAT(A1)
```

would read only the first character of the input. The remaining nine characters of LIST would be set to blank.

The notion of blanks as nulls or zeros has no meaning for characters. The blank is a legitimate character and is treated as meaningful, completely distinct from the notion of a null or a zero.

A simple variant on ch1301 which uses the character variable temp to hold the text between the two numbers appears below:

```
program ch1304
implicit none
integer , parameter :: n=12
integer :: i
integer , dimension(1:n) :: x
integer , dimension(1:n) :: y
character*9 :: temp
  do i=1,n
    read  100,x(i),temp,y(i)
    100 format(2x,i2,a,i3)
    print 200,x(i),y(i)
    200 format(1x,i3,2x,i3)
  end do
end program ch1304
```

Note that in the format statement we just use the A edit descriptor and the number of characters to read is picked up from the variable declaration.

13.5 Skipping spaces and lines

The X format is also useful for input. There may be fields in your data which you do not wish to read. These are easily omitted by the X format:

```
READ(UNIT=*,FMT=100) A,B
100 FORMAT(F10.4,10X,F8.3)
```

Similarly, you can *jump over* or ignore entire records by using the oblique. Do note, however, that

```
READ(UNIT=*,FMT=100) A,B
100 FORMAT(F10.4/F10.4)
```

would read A from one line (or record) and B from the next. To omit a record between A and B, the format would need to be

```
100 FORMAT(F10.4//F10.4)
```

Another way to skip over a record is

```
READ(UNIT=*,FMT=100)
100 FORMAT()
```

with no variable name at all.

13.6 Reading

As you have already seen, reading, or the input of information, is accomplished through the READ statement. We have used

```
READ *,X,Y
```

for list directed input from the terminal, and

```
READ(UNIT=*,FMT=100) X,Y
```

for formatted input from the terminal. These forms may be expanded to

```
READ(UNIT=*,FMT=*) X,Y
```

or

```
READ(UNIT=*,FMT=100) X,Y
```

for input from the terminal, or to

```
READ(UNIT=5,FMT=*) X,Y
```

or

```
READ(UNIT=5,FMT=100) X,Y
```

when we wish to associate the READ statement with a particular unit number (or format label, for formatted input). As with the WRITE statement, these last two READ statements may be abbreviated to

```
READ(5,*) X,Y
```

and

```
READ(5,100) X,Y
```

13.7 File manipulation again

The OPEN and CLOSE statements are also relevant to files which are used as input, and they may be used in the same ways. Besides introducing the notion of manipulating lots of files, the OPEN statement allows you to change the default for the treatment of blanks. The default is to treat blanks as null, but the statement BLANK='ZERO' changes the default to treat blanks as zeros. There are other parameters on the OPEN, which are considered elsewhere.

Once you have OPENed a file, you may not issue another OPEN for the same file until it has been CLOSEd, except in the case of the BLANK= parameter. You may change the default back again with

```
OPEN(UNIT=10,FILE='Example.dat')
READ(UNIT=10,FMT=100) A,B
...
OPEN(UNIT=10,FILE='Example.dat',BLANK='ZERO')
READ(UNIT=10,FMT=100) A,B
```

This implies that, within the same input file, you may treat some records as blank for null, and some as blank for zero. This sounds very dangerous, and is better done by manipulating individual formats if it has to be done at all.

Given that you may write a file, you may also *rewind* it, in order to get back to the beginning. The syntax is similar to the other commands:

```
REWIND(UNIT=1)
```

This often comes in useful as a way of providing backing storage, where intermediate data can be stored on file and then used later in the processing.

The notion of records in Fortran input and output has been introduced. If you are confident in your understanding of this ambiguous and nebulous concept, you can *backspace* through a file, using the statement

```
BACKSPACE(UNIT=1)
```

which moves back over a single record on the designated file. There is no point in trying to BACKSPACE or REWIND if the input is from the keyboard or terminal.

13.8 Reading using array sections

Consider the following output:

```
 50.0  47.0  70.0  89.0  30.0  46.0  =  55.33
 37.0  67.0  85.0  65.0  68.0  98.0  =  70.00
 25.0  45.0  65.0  48.0  10.0  36.0  =  38.17
 89.0  56.0  82.5  45.0  30.0  65.0  =  61.25
 68.0  78.0  95.0  76.0  98.0  65.0  =  80.00
 ====  ====  ====  ====  ====  ====
 53.8  58.6  79.5  64.6  47.2  62.0
```

A program to read this file using array sections is as follows:

```
program ch1305
implicit none
integer , parameter :: nrow=5
integer , parameter :: ncol=6
REAL , DIMENSION(1:nrow,1:ncol) :: Exam_Results     =
0.0
real , dimension(1:nrow)          :: People_average   =
0.0
real , dimension(1:ncol)          :: Subject_Average =
0.0
integer :: r,c
  do r=1,nrow
    read 100,(exam_results(r,1:ncol)),people_average(r)
    100 format(1x,6(1x,f5.1),4x,f6.2)
  end do
  read *
  read 110, subject_average(1:ncol)
  110 format(1x,6(1x,f5.1))
  do r=1,nrow
    print
200,(exam_results(r,c),c=1,ncol),people_average(r)
```

```
      200 format(1x,6(1x,f5.1),'   = ',f6.2)
   end do
   print *,'   ====   ====   ====   ====   ====   ====='
   print 210, subject_average(1:ncol)
   210 format(1x,6(1x,f5.1))
end program ch1305
```

Note also the use of

read *

to skip a line.

If you are on a UNIX or Linux system use diff to compare the input and output files. They should be the same.

13.9 Timing of reading formatted files

A program to read a formatted file is shown below:

```
program ch1306
implicit none
integer , parameter :: n=1000000
integer , dimension(1:n) :: x
real    , dimension(1:n) :: y
integer :: i
real :: t,t1,t2,t3,t4,t5
character*10 :: comment
   open(unit=10,file='ch1306.txt')
   call cpu_time(t)
   t1=t
   comment=' Intial '
   print 100,comment,t1
   do i=1,n
      read(10,200) x(i)
      200 format(1x,i10)
   end do
   call cpu_time(t)
   t2=t-t1
   comment = ' i read '
   print 100,comment,t2
   do i=1,n
      read(10,300) y(i)
      300 format(1x,f10.0)
   end do
```

```
   call cpu_time(t)
   t3=t-t1-t2
   comment = ' r read '
   print 100,comment,t3
   100 format(1x,a,2x,f7.3)
   do i=1,10
     print *,x(i), ' ' , y(i)
   end do
end program ch1306
```

Some timing data from the Intel compiler follows:

```
   Intial         0.063
   i read         1.922
   r read         1.828
              1      1.000000
              2      2.000000
              3      3.000000
              4      4.000000
              5      5.000000
              6      6.000000
              7      7.000000
              8      8.000000
              9      9.000000
             10      10.00000
```

13.10 Timing of reading unformatted files

The following is a program to read from an unformatted file:

```
program ch1307
implicit none
integer , parameter :: n=1000000
integer , dimension(1:n) :: x
real    , dimension(1:n) :: y
integer :: i
real :: t,t1,t2,t3,t4,t5
character*10 :: comment
   open(unit=10,file='ch1307.txt',form='unformatted')
   call cpu_time(t)
   t1=t
   comment=' Intial '
   print 100,comment,t1
   read(10) x
```

```
   call cpu_time(t)
   t2=t-t1
   comment = ' i read '
   print 100,comment,t2
   read (10) y
   call cpu_time(t)
   t3=t-t1-t2
   comment = ' r read '
   print 100,comment,t3
   100 format(1x,a,2x,f7.3)
   do i=1,10
     print *,x(i), ' ' , y(i)
   end do
end program ch1307
```

Some timing data from the Intel compiler follows.

```
   Intial         0.047
   i read         0.063
   r read         0.063
              1      1.000000
              2      2.000000
              3      3.000000
              4      4.000000
              5      5.000000
              6      6.000000
              7      7.000000
              8      8.000000
              9      9.000000
             10      10.00000
```

13.11 Errors when reading

In discussing some aspects of input, it has been pointed out that errors may be made. Where such errors are noticed, in the sense that something illegal is being attempted, there are two options:

- Print a diagnostic message, and allow correction of the mistake.
- Print a diagnostic message, and terminate the program.

The only time that the first makes sense is when you are interacting with a program at a terminal. Some Fortran implementations provide correction facilities in a case like this, but most do not.

Chapter 21 looks at how we handle errors in input data, together with a more in-depth coverage of file I/O.

13.12 Summary

Values may be read in from the keyboard, terminal or from another file through fixed formats.

Much of the structure of input format statements is very similar to that of the output formats. Broadly speaking, data written out in a particular format may be read in by the same format. However, there is greater flexibility, and quite a variety of forms can be accepted on input.

A key distinction to make is the interpretation of blanks, as either nulls or zeros; alternative interpretations can radically alter the structure of the input data.

Fortran allows file names to be associated with unit numbers through the OPEN statement. This statement allows control of the interpretation of blanks, although this can also be done through the BN and BZ formats.

Files can also be manipulated through REWIND and BACKSPACE.

13.13 Problems

1. Write a program that will read in two reals and one integer, using

```
FORMAT(F7.3,I4,F4.1)
```

and that, in one instance treats blanks as zeros and in the second treats them as nulls. Use PRINT * to print the numbers out immediately after reading them in. What do you notice? Can you think of instances where it is necessary to use one rather than the other?

2. Write a program to read in and write out a real number using

```
FORMAT(F7.2)
```

What is the largest number that you can read in and write out with this format? What is the largest negative number that you can read in and write out with this format? What is the smallest number, other than zero, that can be read in and written out?

3. Rewrite two of the earlier programs that used READ,* and PRINT,* to use FORMAT statements.

4. Write a program to read the file created by either the temperature conversion program or the litres and pints conversion program. Make sure that the programs ignore the line printer control characters and any header and title information. This

kind of problem is very common in programming (writing a program to read and possibly manipulate data created by another program).

5. Use the OPEN, REWIND, READ and WRITE statements to input a value (or values) as a character string, write this to a file, rewind the file, read in the values again, this time as real variables with blanks treated as null, and then repeat with blanks as zeros.

6. Demonstrate that input and output formats are not symmetric — i.e., what goes in does not necessarily come out.

7. Can you suggest why Fortran treats blanks as null rather than zero?

8. What happens at your terminal when you enter faulty data, inappropriate for the formats specified? We will look at how we address this problem in Chapter 21.

14

Files

"It is a capital mistake to theorise before one has data."

Sir Arthur Conan Doyle

Aims

The aims of this chapter are:

- To review the process of file creation at a terminal.
- To introduce more formally the idea of the file as a fundamental entity.
- To show how files can be declared explicitly by the OPEN and CLOSE statements.
- To introduce the arguments for the OPEN and CLOSE statements.
- To demonstrate the interaction between the READ/WRITE statements and the OPEN/CLOSE statements.

14 Files

When you work interactively on a terminal, you are working with files, files that contain programs, files that contain data, and perhaps files that are libraries. The file is fundamental to most modern operating systems, and almost all operations are carried out on files.

In this chapter we are going to extend some of your ideas about files. Let us consider what kinds of files you have met so far:

1. Text files. These are the source of your programs, compilation listings, etc. They can be examined by printing them. They can also be transmitted around a computer system fairly easily. A file sent to a printer is a text file. Mail messages are generally plain text files. Note that when mail messages arrive in your mail box they will then typically contain additional nonprintable information.

2. Data files. These exist in two main forms: firstly those prepared by using an editor, (hence a text file) and those prepared using a package or program, in a computer readable form, but not directly readable by a human.

3. Binary, object or relocatable files, e.g., output from the compiler, satellite data. They cannot be printed. To examine files like these you need to use special utilities, provided by most operating systems.

The above categories account for the majority of files that you have met so far.

If you use a word processor then you will also have met files that are textual with additional nonprintable information.

Let us now consider how we can manipulate files using Fortran. They will generally be data files, and will thus be text files. They can therefore be listed, etc., using standard operating system commands.

14.1 Data files in Fortran

These allow us to associate a logical unit number with any arbitrary file name during the running of the program; e.g.,

```
OPEN(UNIT=1,FILE='DATA')
```

would associate the name DATA and the logical unit 1, so that

```
READ(UNIT=1,FMT=100) X
```

would read from DATA. Note that for this to work on some operating systems the file DATA must be *local* to the session; we specify the name as a character variable. If we then wanted to use a subsequent data file, we could have another OPEN

statement, but if we want to use the same logical unit number, we must first CLOSE the file

```
CLOSE(UNIT=1,FILE='DATA')
```

before we

```
OPEN(UNIT=1,FILE='DATA2')
```

In this way we can keep referring to logical unit 1, but change the file associated with it. This can be useful in interactive programs where we wish to analyse different sets of data, e.g.:

```
PROGRAM ch1401
IMPLICIT NONE
REAL :: X
CHARACTER (7) :: WHICH
  OPEN(UNIT=5,FILE='INPUT')
  DO
    WRITE(UNIT=6,FMT='('' DATA SET NAME, OR END'')')
    READ(UNIT=5,FMT='(A)') WHICH
    IF(WHICH == 'END') EXIT
    OPEN(UNIT=1,FILE=WHICH)
    READ(UNIT=1,FMT=100) X
    ...
    CLOSE(UNIT=1,FILE=WHICH)
  END DO
END PROGRAM ch1401
```

One useful feature of the OPEN statement is that there are other parameters. What would happen, for example, if the file is not there? To take care of this you can use the IOSTAT and STATUS keywords, e.g.,

```
OPEN(UNIT=1,FILE='DATA',IOSTAT=FileStat,STATUS='OLD')
```

STATUS can be equated to one of four values:

```
STATUS='OLD'
STATUS='NEW'
STATUS='SCRATCH'
STATUS='UNKNOWN'
```

If we say STATUS='NEW', we are creating a new file and it should not matter whether a file of the same name is present; 'SCRATCH' does not concern us, while 'UNKNOWN' implies that if a file of the correct name is present use it, but if not

create a 'NEW' one. If you omit the STATUS= keyword altogether, the value 'UNKNOWN' will be assumed. If we use STATUS='OLD' and the file is not present, this will cause an error which will be reflected in the value associated with the variable `Open_File_Status`. Consider the following example:

```
...
OPEN(UNIT=1,FILE='DATA',IOSTAT=FileStat,STATUS='OLD')
IF (FileStat > 0) THEN
   PRINT *,' Error opening file, please check'
   STOP
END IF
READ(UNIT=1,FMT=100) X
...
```

The program will terminate after printing an appropriate error message. The standard defines that if an error occurs then IOSTAT will return a positive integer value. A value of zero is returned if there is no error.

14.2 Summary of options on OPEN

UNIT: The unit number of the file to be opened.

IOSTAT: The I/O status specifier designates a variable to store a value indicating the status of a data transfer operation. It takes the following form:

IOSTAT=*i-var*

i-var

is a scalar integer variable. When a data transfer statement is executed, *i-var* is set to one of the following values:

- A positive integer indicating that an error condition occurred.
- A negative integer indicating that an end-of-file or end-of-record condition occurred. The actual values vary between compilers.
- Zero indicating no error, end-of-file, or end-of-record condition occurred.

Execution continues with the statement following the data transfer statement or the statement identified by a branch specifier (if any).

An end-of-file condition occurs only during execution of a sequential READ statement; an end-of-record condition occurs only during execution of a nonadvancing READ statement.

FILE: Character expression specifying the file name.

STATUS: Character expression specifying the file status. It can be one of 'OLD', *'NEW', 'SCRATCH' or 'UNKNOWN'*.

ACCESS: Character expression specifying whether the file is to be used in a sequential or random fashion. Valid values are *SEQUENTIAL* (the default) or *DIRECT*.

The two most common access mechanisms for files are sequential and direct. Consider a file with 1000 records. To get at record 789 in a sequential file means reading or processing the first 788 records. To get at record 789 in a direct access file means using a record number to immediately locate record 789.

FORM: Character expression specifying

FORMATTED if the file is opened for formatted I/O

or

UNFORMATTED if the file is opened for unformatted I/O

The default is formatted for sequential access files and unformatted for direct access files. If the file exists, FORM must be consistent with its present characteristics.

As noted earlier data are maintained internally in a binary format, not immediately comprehensible by humans. When we wish to look at the data we must write it in a formatted fashion, i.e., as a sequence of printable ASCII characters — text, or the written word. This formatting will carry with it an overhead in terms of the time required to do it. It will also carry with it the penalty of conversion from one number base (internally binary) to another and also loss of significance due to rounding with whatever edit descriptors are used, e.g., writing out as F7.4.

If we are interested in reusing data on the same system and compiler then we can use the unformatted option and avoid both the time overhead (as there is no conversion between the internal and external formats) and the loss of significance associated with formatted data.

Please note that unformatted files are rarely portable between different computer systems, and sometimes even between different compilers on the same system.

We will look again at the use of unformatted files in Chapter 28 when we deal with efficiency and the space-time trade-off.

RECL: Integer variable or constant specifying the record length for a direct access file. It is specified in characters for a formatted file and words for an unformatted file.

BLANK: Character expression having one of the following values:

'NULL' if blanks are to be ignored on reading. Note that a field of all blanks is treated as 0!

'ZERO' if blanks are to be treated as zeros.

14.3 More foolproof I/O

Fortran provides a way of writing more foolproof programs involving I/O. This is done via the IOSTAT keyword on the READ statement. Consider the following:

```
PROGRAM ch1402
IMPLICIT NONE
INTEGER :: IO_Stat_Number=-1
INTEGER :: I
  DO
    READ (UNIT=*,FMT=10,&
     IOSTAT=IO_Stat_Number) I
    10 FORMAT(I3)
    PRINT *,' iostat=',IO_Stat_Number
    PRINT *,I
    IF (IO_Stat_Number==0) EXIT
  END DO
END PROGRAM ch1402
```

The following data input should be tried and the values of IO_Stat_Number should be examined

- A valid three-digit number + [RETURN] key
- A three-digit number with an embedded blank, e.g., 1 2 + [RETURN] key
- [RETURN] key only
- [CTRL] + Z
- Any other nonnumeric character on the keyboard
- 100200300 + [RETURN] key
- [CTRL] + C

This will then enable you to write programs that handle common I/O errors.

Consider the following:

```
PROGRAM ch1403
INTEGER , DIMENSION(10) :: A =&
  (/-1,-1,-1,-1,-1,-1,-1,-1,-1,-1/)
INTEGER :: IO_Stat_Number=0
INTEGER :: I
  OPEN(UNIT=1,FILE='DATA.DAT',STATUS='OLD')
```

```
   DO I=1,10
      READ (UNIT=1,FMT=10,IOSTAT=IO_Stat_Number) A(I)
      10 FORMAT(I3)
      IF (IO_Stat_Number == 0) THEN
          CYCLE
      ELSEIF (IO_Stat_Number == -1) THEN
         PRINT *,' End of file detected at line ',I
         PRINT *,' Please check data file'
         EXIT
      ELSEIF (IO_Stat_Number  > 0 ) THEN
         PRINT *,' Non numeric data at line ',I
         PRINT *,' Please correct data file'
         EXIT
      ENDIF
   END DO
   DO I=1,10
      PRINT * , ' I = ',I,' A(I) = ',A(I)
   ENDDO
END PROGRAM ch1403
```

The above program is system specific but interestingly the following compilers return the same value for end of file. They return different values for nonnumeric data:

- NAG/Salford compiler.
- DEC Alpha OPENVMS compiler.
- NagAce Fortran 90 under Solaris.
- Sun F90 compiler (release 2.x).
- Nag F95 compiler under Solaris.
- Compaq/Dec F95, 6.01A.

What happens with a completely blank line?

Note that in the above example the testing for the various conditions only exits the DO loop for reading data from the file. This means that execution would continue with the statement immediately after the END DO statement. This may not be what we want in all cases, and the EXIT may be replaced with a STOP statement to terminate execution immediately.

14.4 Summary

The file is a fundamental entity within the operating system.

A file may be manipulated in Fortran by associating its name with a unit number. All subsequent communication within the program is through the unit number.

When a file is opened there are a large number of equatable keywords which may be employed to establish its characteristics.

The default file type used in Fortran is *sequential formatted,* but several other esoteric types may be used.

14.5 Problems

1. Write a program to write the first 500 integers to a file using formatted I/O. Put 10 values on a line, with a blank as the first character of the line, and eight columns allowed for each integer, with two spaces between integer fields.

Now write a program to read this file into an array, and write the numbers in reverse order over the original data, i.e., the data file now contains the first 500 numbers in descending order.

Now modify the first program to add the next 500 integers to the same file, so that the file now comprises the first 500 numbers in descending order, and the next 500 numbers in ascending order.

2. To write and maintain a crude database of student details, we might do the following: create separate files for each year — CLAS1, CLAS2, CLAS3, or COF84, COF85, COF86, and so on. In either case there is an unchanging prefix, CLAS or COF, and a variable suffix, which identifies membership within the overall group. In each of the files we may wish to record details like name, date of birth, address, courses taken, etc. Such files will require updating as details change or as errors are noted. Write (or sketch out) a program which would select and maintain such records and would allow corrected files to be printed out. While you might feel that the most appropriate tool for this job is an editor, you might find it too powerful a tool. An editor can leave files in a sorry state. Naturally, any program like this should be helpful (so called '*user friendly*'). Is this sort of information sensitive enough to require security checks and passwords?

15

Functions

"I can call spirits from the vasty deep.
Why so can I, or so can any man; but will they come
when you do call for them?"

William Shakespeare, *King Henry IV, part 1*

Aims

The aims of this chapter are:

- To consider some of the reasons for the inclusion of functions in a programming language.
- To introduce, with examples, some of the predefined functions available in Fortran 95.
- To introduce a classification of intrinsic functions, generic, elemental, transformational.
- To introduce the concept of a user defined function.
- To introduce the concept of a recursive function.
- To introduce the concept of user defined elemental and pure functions.
- To briefly look at scope rules in Fortran 95 for variables and functions.
- To look at internal user defined functions.

15 Functions

The role of functions in a programming language and in the problem-solving process is considerable and includes:

- Allowing us to refer to an action using a meaningful name, e.g., SINE(X) a very concrete use of abstraction.
- Providing a mechanism that allows us to break a problem down into parts, giving us the opportunity to structure our problem solution.
- Providing us with the ability to concentrate on one part of a problem at a time and ignore the others.
- Allowing us to avoid the replication of the same or very similar sections of code when solving the same or a similar subproblem which has the secondary effect of reducing the memory requirements of the final program.
- Allowing us to build up a library of functions or modules for solving particular subproblems, both saving considerable development time and increasing our effectiveness and productivity.

Some of the underlying attributes of functions are:

- They take parameters or arguments.
- The parameter can be an expression.
- A function will normally return a value and the value returned is normally dependent on the parameter(s).
- They can sometimes take arguments of a variety of types.

Most languages provide both a range of predefined functions and the facility to define our own. We will look at the predefined functions first.

15.1 An introduction to predefined functions and their use

Fortran provides over a hundred intrinsic functions and subroutines. For the purposes of this chapter a subroutine can be regarded as a variation on a function. Subroutines are covered in more depth in a later chapter. They are used in a straightforward way. If we take the common trigonometric functions, sine, cosine and tangent, the appropriate values can be calculated quite simply by:

```
X=SIN(Y)
Z=COS(Y)
A=TAN(Y)
```

This is in rather the same way that we might say that X is a function of Y, or X is sine Y. Note that the argument, Y, is in *radians* not *degrees*.

15.1.1 Example 1: Simple function usage

A complete example is given below:

```
PROGRAM ch1501
REAL :: X
   PRINT *,' Type in an angle (in radians)'
   READ *,X
   PRINT *,' Sine of ', X ,' = ',SIN(X)
END PROGRAM ch1501
```

These functions are called *intrinsic functions.* A selection is follows:

Function	Action	Example
INT	conversion to integer	J=INT(X)
REAL	conversion to real	X=REAL(J)
ABS	absolute value	X=ABS(X)
MOD	remaindering remainder when I divided by J	K=MOD(I,J)
SQRT	square root	X=SQRT(Y)
EXP	exponentiation	Y=EXP(X)
LOG	natural logarithm	X=LOG(Y)
LOG10	common logarithm	X=LOG10(Y)
SIN	sine	X=SIN(Y)
COS	cosine	X=COS(Y)
TAN	tangent	X=TAN(Y)
ASIN	arcsine	Y=ASIN(X)
ACOS	arccosine	Y=ACOS(X)
ATAN	arctangent	Y=ATAN(X)
ATAN2	arctangent(a/b)	Y=ATAN2(A,B)

A complete list is given in Appendix D.

15.2 Generic functions

All but four of the intrinsic functions and procedures are generic, i.e., they can be called with arguments of one of a number of kind types.

15.2.1 Example 2: The ABS generic function

The following short program illustrates this with the ABS intrinsic function:

```
PROGRAM ch1502
IMPLICIT NONE
COMPLEX :: C=(1,1)
REAL    :: R=10.9
INTEGER :: I=-27
  PRINT *,ABS(C)
  PRINT *,ABS(R)
  PRINT *,ABS(I)
END PROGRAM ch1502
```

The four nongeneric functions are LGE, LGT, LLE and LLT — the lexical character comparison functions.

Type this program in and run it on the system you use.

It is now possible with Fortran 95 for the arguments to the intrinsic functions to be arrays. It is convenient to categorise the functions into either elemental or transformational, depending on the action performed on the array elements.

15.3 Elemental functions

These functions work with both scalar and array arguments, i.e., with arguments that are either single or multiple valued.

15.3.1 Example 3: Elemental function use

Taking the earlier example with the evaluation of sine as a basis, we have:

```
PROGRAM ch1503
REAL , DIMENSION(5) :: X = (/1.0,2.0,3.0,4.0,5.0/)
  PRINT *,' Sine of ', X ,' = ',SIN(X)
END PROGRAM ch1503
```

In the above example the sine function of each element of the array X is calculated and printed.

15.4 Transformational functions

Transformational functions are those whose arguments are arrays, and work on these arrays to transform them in some way.

15.4.1 Example 4: Simple transformational use

To highlight the difference between an element-by-element function and a transformational function consider the following examples:

```
PROGRAM ch1504
IMPLICIT NONE
REAL , DIMENSION(5) :: X = (/1.0,2.0,3.0,4.0,5.0/)
! Elemental function
   PRINT *,' Sine of ', X ,' = ',SIN(X)
! Transformational function
   PRINT *,' Sum of ', X ,' = ',SUM(X)
END PROGRAM ch1504
```

The SUM function adds each element of the array and returns the SUM as a scalar, i.e., the result is single valued and not an array.

15.4.2 Example 5: Intrinsic DOT_PRODUCT use

The following program uses the transformational function DOT_PRODUCT:

```
PROGRAM ch1505
IMPLICIT NONE
REAL , DIMENSION(5) :: X = (/1.0,2.0,3.0,4.0,5.0/)
   PRINT *,' Dot product of X with X is'
   PRINT *,' ',DOT_PRODUCT(X,X)
END PROGRAM ch1505
```

Try typing these examples in and running them to highlight the differences between elemental and transformational functions.

15.5 Notes on function usage

You should not use variables which have the same name as the intrinsic functions; e.g., what does SIN(X) mean when you have declared SIN to be a real array?

When a function has multiple arguments care must be taken to ensure that the arguments are in the correct position and of the appropriate kind type.

You may also replace arguments for functions by expressions, e.g.,

```
X = LOG(2.0)
```

or

```
X = LOG(ABS(Y))
```

or

```
X = LOG(ABS(Y)+Z/2.0)
```

15.6 Example 6: Easter

This example uses only one function, the MOD (or modulus). It is used several times, helping to emphasise the usefulness of a convenient, easily referenced function. The program calculates the date of Easter for a given year. It is derived from an algorithm by Knuth, who also gives a fuller discussion of the importance of its algorithm. He concludes that the calculation of Easter was a key factor in keeping arithmetic alive during the Middle Ages in Europe. Note that determination of the Eastern churches' Easter requires a different algorithm:

```
PROGRAM ch1506
IMPLICIT NONE
INTEGER :: Year, Metcyc, Century, Error1, Error2, Day
INTEGER :: Epact, Luna, Temp
! A program to calculate the date of Easter
   PRINT *,' Input the year for which Easter'
   PRINT *,' is to be calculated'
   PRINT *,' enter the whole year, e.g. 1978 '
   READ *,Year
! calculating the year in the 19 year
! metonic cycle using variable metcyc
   Metcyc = MOD(Year,19)+1
   IF(Year <= 1582)THEN
      Day = (5*Year)/4
      Epact = MOD(11*Metcyc-4,30)+1
   ELSE
!         calculating the Century-century
      Century = (Year/100)+1
!          accounting for arithmetic inaccuracies
!          ignores leap years etc.
      Error1 = (3*Century/4)-12
      Error2 = ((8*Century+5)/25)-5
!          locating Sunday
      Day = (5*Year/4)-Error1-10
!          locating the epact(full moon)
      Temp = 11 * Metcyc + 20 + Error2 - Error1
      Epact = MOD(Temp,30)
      IF(Epact <= 0) THEN
         Epact = 30 + Epact
```

```
      ENDIF
      IF((Epact == 25 .AND. Metcyc > 11) &
      .or. Epact == 24)THEN
         Epact = Epact+1
      ENDIF
   ENDIF
!      finding the full moon
   Luna= 44 - epact
   IF (Luna < 21) THEN
      Luna = Luna+30
   ENDIF
!      locating Easter Sunday
   Luna = Luna+7-(MOD(Day+Luna,7))
!      locating the correct month
   IF(Luna > 31)THEN
      Luna = Luna - 31
      PRINT *,' for the year ',YEAR
      PRINT *,' Easter falls on April ',Luna
   ELSE
      PRINT *,' for the year ',YEAR
      PRINT *,' Easter falls on march ',Luna
   ENDIF
END PROGRAM ch1506
```

We have introduced a new statement here, the IF THEN ENDIF, and a variant the IF THEN ELSE ENDIF. A more complete coverage is given in the chapter on control structures. The main point of interest is that the normal sequential flow from top to bottom can be varied. In the following case,

IF (expression) THEN

block of statements

ENDIF

if the expression is true the block of statements between the IF THEN and the ENDIF is executed. If the expression is false then this block is skipped, and execution proceeds with the statements immediately after the ENDIF.

In the following case,

IF (expression) THEN

block 1

ELSE

block 2

ENDIF

if the expression is true block 1 is executed and block 2 is skipped. If the expression is false then block 2 is executed and block 1 is skipped. Execution then proceeds normally with the statement immediately after the ENDIF.

As well as noting the use of the MOD generic function in this program, it is also worth noting the structure of the decisions. They are *nested*, rather like the nested DO loops we met earlier.

15.7 Complete list of predefined functions

Due to the large number of predefined functions it is useful to classify them, and the following is one classification.

15.7.1 Inquiry functions

These functions return information about their arguments. They can be further subclassified into BIT, CHARACTER, NUMERIC, ARRAY, POINTER, ARGUMENT PRESENCE:

Bit	BIT_SIZE
Character	LEN
Numeric	DIGITS, EPSILON, EXPONENT, FRACTION, HUGE, KIND, MAXEXPONENT, MINEXPONENT, NEAREST, PRECISION, RADIX, RANGE, RRSPACING, SCALE, SET_EXPONENT, SELECTED_INT_KIND, SELECTED_REAL_KIND, SPACING, TINY
Array	ALLOCATED, LBOUND, SHAPE, SIZE, UBOUND,
Pointer	ASSOCIATED, NULL
Argument Presence	PRESENT

15.7.2 Transfer and conversion functions

These functions convert data from one type and kind type to another type and kind type. Most of them are by necessity generic.

Transfer and Conversion ACHAR, AIMAG, AINT, ANINT, CHAR, CMPLX, CONJG, DBLE, IACHAR, IBITS, ICHAR, INT, LOGICAL, NINT, REAL, TRANSFER

15.7.3 Computational functions

These functions actually carry out a computation of some sort and return the result of that computation:

Numeric ABS, ACOS, ASIN, ATAN, ATAN2, CEILING, COS, COSH, DIM, DOT_PRODUCT, DPROD, EXP, FLOOR, LOG, LOG10, MATMUL, MAX, MIN, MOD, MODULO, SIGN, SIN, SINH, SQRT, TAN, TANH

Character ADJUSTL, ADJUSTR, INDEX, LEN_TRIM, LGE, LGT, LLE, LLT, REPEAT, SCAN, TRIM, VERIFY

Bit BTEST, IAND, IBCLR, IBSET, IEOR, IOR, ISHFT, ISHFTC, NOT

15.7.4 Array functions

Reduction ALL, ANY, COUNT, MAXVAL, MINVAL, PRODUCT, SUM

Construction MERGE, PACK, SPREAD, UNPACK

Reshape RESHAPE

Manipulation CSHIFT, EOSHIFT, TRANSPOSE

Location MAXLOC, MINLOC

15.7.5 Predefined subroutines

Date and Time CPU_TIME, DATE_AND_TIME, SYSTEM_CLOCK

Random Number RANDOM_NUMBER, RANDOM_SEED

Other MVBITS

An alphabetical list of all intrinsic functions and procedures is given in Appendix D. This list provides the following information:

- Function name.
- Description.
- Argument name and type.
- Result type.
- Classification.
- Examples of use.

Appendix D should be consulted for a more complete and thorough understanding of intrinsic functions and their use in Fortran 95.

15.8 Supplying your own functions

There are two stages here: firstly, to define the function and, secondly, to reference or use it. Consider the calculation of the greatest common divisor of two integers.

15.8.1 Example 7: Simple user defined function

The following defines a function to achieve this:

```
INTEGER FUNCTION GCD(A,B)
IMPLICIT NONE
INTEGER , INTENT(IN) :: A,B
INTEGER :: Temp
   IF (A < B) THEN
     Temp=A
   ELSE
     Temp=B
   ENDIF
   DO WHILE ((MOD(A,Temp) /= 0) .OR. (MOD(B,Temp) /=0))
     Temp=Temp-1
   END DO
   GCD=Temp
END FUNCTION GCD
```

To use this function, you reference or call it with a form like:

```
PROGRAM ch1507
IMPLICIT NONE
INTEGER :: I,J,Result
INTEGER :: GCD
```

```
   PRINT *,' Type in two integers'
   READ *,I,J
   Result=GCD(I,J)
   PRINT *,' GCD is ',Result
END PROGRAM ch1507
```

The first line of the function

```
INTEGER FUNCTION GCD(A,B)
```

has a number of items of interest:

- Firstly the function has a type, and in this case the function is of type INTEGER, i.e., it will return an integer value.
- The function has a name, in this case GGD.
- The function takes arguments or parameters, in this case A and B.

The structure of the rest of the function is the same as that of a program, i.e., we have declarations, followed by the executable part. This is because both a program and a function can be regarded as a so-called *program unit*. We will look into this more fully in later chapters.

In the declaration we also have a new attribute for the INTEGER declaration. The two parameters A and B are of type integer, and the INTENT(IN) attribute means that these parameters will NOT be altered by the function.

The value calculated is returned through the function name somewhere in the body of the executable part of the function. In this case GCD appears on the left-hand side of an arithmetic assignment statement at the bottom of the function. The end of the function is signified in the same way as the end of a program:

```
END FUNCTION GCD
```

We then have the program which actually uses the function GCD. In the program the function is called or invoked with I and J as arguments. The variables are called A and B in the function, and references to A and B in the function will use the values that I and J have respectively in the main program. We will look into the whole area of argument association in much greater depth in later chapters.

Note also a new control statement, the DO WHILE ENDDO. In the following case,

DO WHILE (expression)

  block of statements

```
ENDDO
```

the block of statements between the DO WHILE and the ENDDO is executed whilst the expression is true. There is a more complete coverage in Chapter 16.

We have two options here regarding compilation. Firstly, to make the function and the program into one file, and invoke the compiler once. Secondly, to make the function and program into separate files, and invoke the compiler twice, once for each file. With large programs comprising one program and several functions it is probably worthwhile to keep the component parts in different files and compile individually, whereas if it consists of a simple program and one function then keeping things together in one file makes sense.

Try this program out on the system you work with.

15.9 An introduction to the scope of variables and local variables

One of the major strengths of Fortran is the ability to work on parts of a problem at a time. This is achieved by the use of *program units* (a main program, one or more functions and one or more subroutines) to solve discrete subproblems. Interaction between them is limited and can be isolated, for example, to the arguments of the function. Thus variables in the main program can have the same name as variables in the function and they are completely separate variables, even though they have the same name. Thus we have the concept of a local variable in a program unit. We will look into this area again after a coverage of recursion and very thoroughly after the coverage of subroutines and modules.

In the example above I, J, Result, are local to the main program. The declaration of GCD is to tell the compiler that it is an integer, and in this case it is an external function.

A and B in the function GCD do not exist in any real sense; rather they will be replaced by the actual variable values from the calling routine, in this case by whatever values I and J have. Temp is local to GCD.

15.10 Recursive functions

There is an additional form of the function header that must be used when the function is recursive. Recursion means the breaking down of a problem into a simpler but identical subproblem. The concept is best explained with reference to an actual example. Consider the evaluation of a factorial, e.g., 5!. From simple mathematics we know that the following is true:

5!=5*4!

4!=4*3!

3!=3*2!

2!=2*1!

1!=1

and thus 5! = 5*4*3*2*1 or 120.

15.10.1 Example 8: Recursive factorial evaluation

Let us look at a program with recursive function to solve the evaluation of factorials.

```
PROGRAM ch1508
IMPLICIT NONE
INTEGER :: I, F, Factorial
   PRINT *,' Type in the number, integer only'
   READ *,I
   DO WHILE(I<0)
      PRINT *,' Factorial only defined for '
      PRINT *,' positive integers: Re-input'
      READ *,I
   END DO
   F=Factorial(I)
   PRINT *,' Answer is', F
END PROGRAM ch1508

RECURSIVE INTEGER FUNCTION Factorial(I) RESULT(Answer)
IMPLICIT NONE
INTEGER , INTENT(IN):: I
   IF (I==0) THEN
      Answer=1
   ELSE
      Answer=I*Factorial(I-1)
   END IF
END FUNCTION Factorial
```

What additional information is there? Firstly, we have an additional attribute on the function header that declares the function to be recursive. Secondly, we must return the result in a variable, in this case Answer. Let us look now at what happens when we compile and run the whole program (both function and main program). If we type in the number 5 the following will happen:

- The function is first invoked with argument 5. The ELSE block is then taken and the function is invoked again.

- The function now exists a second time with argument 4. The ELSE block is then taken and the function is invoked again.
- The function now exists a third time with argument 3. The ELSE block is then taken and the function is invoked again.
- The function now exists a fourth time with argument 2. The ELSE block is then taken and the function is invoked again.
- The function now exists a fifth time with argument 1. The ELSE block is then taken and the function is invoked again.
- The function now exists a sixth time with argument 0. The IF BLOCK is executed and Answer=1. This invocation ends and we return to the previous level, with Answer=1*1.
- We return to the previous invocation and now Answer=2*1.
- We return to the previous invocation and now Answer=3*2.
- We return to the previous invocation and now Answer=4*6.
- We return to the previous invocation and now Answer=5*24.

The function now terminates and we return to the main program or calling routine. The answer 120 is the printed out.

Add a PRINT *,I statement to the function after the last declaration and type the program in and run it. Try it out with 5 as the input value to verify the above statements.

Recursion is a very powerful tool in programming, and remarkably simple solutions to quite complex problems are possible using recursive techniques. We will look at recursion in much more depth in the later chapters on dynamic data types, and subroutines and modules.

15.11 Example 9: Recursive version of GCD

The following is another example of the earlier GCD function but with the algorithm in the function replaced with an alternate recursive solution:

```
PROGRAM ch1509
IMPLICIT NONE
INTEGER :: I,J,Result
INTEGER :: GCD
   PRINT *,' Type in two integers'
   READ *,I,J
   Result=GCD(I,J)
   PRINT *,' GCD is ',Result
```

```
END PROGRAM ch1509

RECURSIVE INTEGER FUNCTION GCD(I,J) RESULT(Answer)
IMPLICIT NONE
INTEGER , INTENT(IN) :: I,J
   IF (J==0) THEN
      Answer=I
   ELSE
      Answer=GCD(J,MOD(I,J))
   ENDIF
END FUNCTION GCD
```

Try this program out on the system you work with, look at the timing information provided, and compare the timing with the previous example. The algorithm is a much more efficient algorithm than in the original example, and hence should be much faster. On one system there was a twentyfold decrease in execution time between the two versions.

Recursion is sometimes said to be inefficient, and the following example looks at a nonrecursive version of the second algorithm.

15.12 Example 10: After removing recursion

The following is a variant of the above, with the same algorithm, but with the recursion removed:

```
PROGRAM ch1510
IMPLICIT NONE
INTEGER :: I,J,Result
INTEGER :: GCD
   PRINT *,' Type in two integers'
   READ *,I,J
   Result=GCD(I,J)
   PRINT *,' GCD is ',Result
END PROGRAM ch1510

INTEGER FUNCTION GCD(I,J)
IMPLICIT NONE
INTEGER , INTENT(INOUT) :: I,J
INTEGER :: Temp
   DO WHILE (J/=0)
      Temp=MOD(I,J)
      I=J
      J=Temp
```

```
   END DO
   GCD=I
END FUNCTION GCD
```

15.13 Pure functions

Within the world of mathematics there is the concept of a pure function. This means that the function only returns a value, and has no effect on the arguments. Fortran 95 introduced the ability to write user defined pure functions. We will provide examples in Chapter 26, when we have covered the additional syntax that is required.

15.14 Elemental functions

Fortran 77 introduced the concept of generic intrinsic functions. Fortran 90 added elemental intrinsic functions and the ability to write generic user defined functions. Fortran 95 squares the circle and enables us to write elemental user defined functions. We will show how this can be done in Chapter 26 when we have covered the additional syntax that is required.

15.15 Internal functions

An internal function is a more restricted and hidden form of the normal function definition.

Since the internal function is specified within a program segment, it may only be used within that segment and cannot be referenced from any other functions or subroutines, unlike the intrinsic or other user defined functions.

15.15.1 Example 11: Stirling's approximation

In this example we use Stirling's approximation for large n,

$$n! = \sqrt{2\pi n}\left(\frac{n}{e}\right)^n$$

and a complete program to use this internal function is given below:

```
PROGRAM ch1511
IMPLICIT NONE
REAL :: Result,N,R
   PRINT *,' Type in N and R'
   READ *,N,R
! NUMBER OF POSSIBLE COMBINATIONS THAT CAN
! BE FORMED WHEN
! R OBJECTS ARE SELECTED OUT OF A GROUP OF N
```

```
! N!/R!(N-R)!
   Result=Stirling(N)/(Stirling(R)*Stirling(N-R))
   PRINT *,Result
   PRINT *,N,R
CONTAINS
REAL FUNCTION Stirling (X)
   REAL , INTENT(IN) :: X
   REAL , PARAMETER :: PI=3.1415927, E =2.7182828
   Stirling=SQRT(2.*PI*X) * (X/E)**X
END FUNCTION Stirling
END PROGRAM ch1511
```

The difference between this example and the earlier ones lies in the CONTAINS statement. The function is now an integral part of the program and could not, for example, be used elsewhere in another function. This provides us with a very powerful way of information hiding and making the construction of larger programs more secure and bug free.

15.16 Resumé

There are a large number of Fortran supplied functions and subroutines (intrinsic functions) which extend the power and scope of the language. Some of these functions are of *generic* type, and can take several different types of arguments. Others are restricted to a particular type of argument. Appendix D should be consulted for a fuller coverage concerning the rules that govern the use of the intrinsic functions and procedures.

When the intrinsic functions are inadequate, it is possible to write *user defined* functions. Besides expanding the scope of computation, such functions aid in problem visualisation and logical subdivision, may reduce duplication, and generally help in avoiding programming errors.

In addition to separately defined user functions, internal functions may be employed. These are functions which are used within a program segment.

Although the normal exit from a user defined function is through the END, other, *abnormal,* exits may be defined through the RETURN statement.

Communication with nonrecursive functions is through the function name and the function arguments. The function *must* contain a reference to the function name on the left-hand side of an assignment. Results may also be returned through the argument list.

We have also covered briefly the concept of scope for a variable, local variables, and argument association. This area warrants a much fuller coverage and we will do this after we have covered subroutines and modules.

15.17 Function syntax

The syntax of a function is:

[function prefix] function_statement &

[RESULT (Result_name)]

[specification part]

[execution_part]

[internal sub program part]

END [FUNCTION [function name]]

and prefix is:

[type specification] RECURSIVE

or

[RECURSIVE] type specification

and the function_statement is:

FUNCTION function_name ([dummy argument name list])

[ ] represent optional parts to the specification.

15.18 Rules and restrictions

The type of the function must only be specified once, either in the function statement or in a type declaration.

The names must match between the function header and END FUNCTION function name statement.

If there is a RESULT clause, that name must be used as the result variable, so all references to the function name are recursive calls.

The function name must be used to return a result when there is no RESULT clause.

We will look at additional rules and restrictions in later chapters.

15.19 Problems

1. Find out the action of the MOD function when one of the arguments is negative. Write your own modulus function to return only a positive remainder. Don't call it MOD!

2. Create a table which gives the sines, cosines and tangents for –1 to 91 degrees in 1 degree intervals. Remember that the arguments have to be in radians. What value will you give π? One possibility is π=4*atan(1.0). Pay particular attention to the following angle ranges:

- –1,0,+1
- 29,30,31
- 44,45,46
- 59,60,61
- 89,90,91

What do you notice about sine and cosine at 0 and 90 degrees? What do you notice about the tangent of 90 degrees? Why do you think this is?

Use a calculator to evaluate the sine, cosine at 0 and 90 degrees. Do the same for the tangent at 90 degrees. Does this surprise you?

Repeat using a spreadsheet, e.g., Excel.

Are you surprised?

Repeat the Fortran program using one or more real kind types.

3. Write a program that will read in the lengths *a* and *b* of a right-angled triangle and calculate the hypotenuse *c*. Use the Fortran SQRT intrinsic.

4. Write a program that will read in the lengths *a* and *b* of two sides of a triangle and the angle between them θ (in degrees). Calculate the length of the third side *c* using the cosine rule:

$$c^2 = a^2 + b^2 - 2abcos(\theta)$$

5. Write a function to convert an integer to a binary character representation. It should take an integer argument and return a character string that is a sequence of zeros and ones. Use the program in Chapter 8 as a basis for the solution.

15.20 Bibliography

Abramowitz M., Stegun I., *Handbook of Mathematical Functions*, Dover, 1968.

- This book contains a fairly comprehensive collection of numerical algorithms for many mathematical functions of varying degrees of obscurity. It is a widely used source.

Association of Computing Machinery (ACM)

- *Collected Algorithms*, 1960–1974

- *Transactions on Mathematical Software*, 1975 —
  A good source of more specialied algorithms. Early algorithms tended to be in Algol, Fortran now predominates.

15.20.1 Recursion and problem solving

The following are a number of books that look at the role of recursion in problem solving and algorithms.

Hofstader D. R., *Gödel, Escher, Bach — an Eternal Golden Braid*, Harvester Press.

- The book provides a stimulating coverage of the problems of paradox and contradiction in art, music and mathematics using the works of Escher, Bach and Gödel, and hence the title. There is a whole chapter on recursive structures and processes. The book also covers the work of Church and Turing, both of whom have made significant contributions to the theory of computing.

Kruse R.L., *Data Structures and Program Design*, Prentice-Hall, 1994.

- Quite a gentle introduction to the use of recursion and its role in problem solving. Good choice of case studies with explanations of solutions. Pascal is used.

Sedgewick R., *Algorithms in Modula 3*, Addison-Wesley, 1993.

- Good source of algorithms. Well written. The GCD algorithm was taken from this source.

Vowels R.A., *Algorithms and Data Structures in F and Fortran,* Unicomp, 1998.

- The only book currently that uses Fortran 90/95 and F. Visit the Fortran web site for more details. They are the publishers.

  http://www.fortran.com/fortran/market.html

Wirth N., *Algorithms + Data Structures = Programs*, Prentice-Hall, 1976.

- In the context of this chapter the section on recursive algorithms is a very worthwhile investment in time.

Wood D., *Paradigms and Programming in Pascal*, Computer Science Press.

- Contains a number of examples of the use of recursion in problem solving. Also provides a number of useful case studies in problem solving.

16

Control Structures

"Summarizing: as a slow-witted human being I have a very small head and I had better learn to live with it and to respect my limitations and give them full credit, rather than try to ignore them, for the latter vain effort will be punished by failure."

Edsger W. Dijkstra, *Structured Programming*

Aims

The aims of this chapter are to introduce:

- Selection among various courses of action as part of the algorithm.
- The concepts and statements in Fortran needed to support the above:
  - Logical expressions and logical operators.
  - One or more *blocks* of statements.
- The IF THEN ENDIF construct.
- The IF THEN ELSE IF ENDIF construct.
- To introduce the CASE statement with examples.
- To introduce the DO loop, in three forms with examples, in particular:
  - The iterative DO loop.
  - The DO WHILE form.
  - The DO ... IF THEN EXIT END DO or repeat until form.
  - The CYCLE statement.
  - The EXIT statement.

16 Control Structures

When we look at this area it is useful to gain some historical perspective concerning the control structures that are available in a programming language.

At the time of the development of Fortran in the 1950s there was little theoretical work around and the control structures provided were very primitive and closely related to the capability of the hardware.

At the time of the first standard in 1966 there was still little published work regarding structured programming and control structures. The seminal work by Dahl, Dijkstra and Hoare was not published until 1972.

By the time of the second standard there was a major controversy regarding languages with poor control structures like Fortran which essentially were limited to the GOTO statement. The facilities in the language had led to the development and continued existence of major code suites that were unintelligible, and the pejorative term *spaghetti* was applied to these programs. Developing an understanding of what a program did became an almost impossible task in many cases.

Fortran missed out in 1977 on incorporating some of the more modern and intelligible control structures that had emerged as being of major use in making code easier to understand and modify.

It was not until the 1990 standard that a reasonable set of control structures had emerged and became an accepted part of the language. The more inquisitive reader is urged to read at least the work by Dahl, Dijkstra and Hoare to develop some understanding of the importance of control structures and the role of structured programming. The paper by Knuth is also highly recommended as it provides a very balanced coverage of the controversy of earlier times over the GOTO statement.

16.1 Selection among courses of action

In most problems you need to choose among various courses of action, e.g.,

- If overdrawn, then do not draw money out of the bank.
- If Monday, Tuesday, Wednesday, Thursday or Friday, then go to work.
- If Saturday, then go to watch Queens Park Rangers.
- If Sunday, then lie in bed for another two hours.

As most problems involve selection between two or more courses of action it is necessary to have the concepts to support this in a programming language. Fortran has a variety of selection mechanisms, some of which are introduced below.

16.1.1 The BLOCK IF statement

The following short example illustrates the main ideas:

```
. wake up
.
. check the date and time
IF (Today = = Sunday) THEN
        .
        . lie in bed for another two hours
        .
ENDIF
.
. get up
. make breakfast
```

If today is Sunday then the block of statements between the IF and the ENDIF is executed. After this block has been executed the program continues with the statements after the ENDIF. If today is not Sunday the program continues with the statements after the ENDIF immediately. This means that the statements after the ENDIF are executed whether or not the expression is true. The general form is:

```
IF (Logical expression) THEN
        .
        Block of statements
        .
ENDIF
```

The logical expression is an expression that will be either true or false; hence its name. Some examples of logical expressions are given below:

```
(Alpha >= 10.1)
```

Test if Alpha is greater than or equal to 10.1

```
(Balance <= 0.0)
```

Test if overdrawn

```
(( Today == Saturday).OR.( Today == Sunday))
```

Test if today is Saturday or Sunday

```
((Actual - Calculated) <= 1.0E-6)
```

Test if Actual minus Calculated is less than or equal to 1.0E-6

Fortran has the following relational and logical operators:

Operator	Meaning	Type
= =	Equal	Relational
/=	Not equal	Relational
>=	Greater than or equal	Relational
<=	Less than or equal	Relational
<	Less than	Relational
>	Greater than	Relational
.AND.	And	Logical
.OR.	Or	Logical
.NOT.	Not	Logical

The first six should be self-explanatory. They enable expressions or variables to be compared and tested. The last three enable the construction of quite complex comparisons, involving more than one test; in the example given earlier there was a test to see whether today was Saturday or Sunday.

Use of logical expressions and logical variables (something not mentioned so far) is covered again in a later chapter on logical data types.

The 'IF *expression* THEN *statements* ENDIF' is called a BLOCK IF construct. There is a simple extension to this provided by the ELSE statement. Consider the following example:

```
IF (Balance > 0.0) THEN
        . draw money out of the bank
ELSE
        . borrow money from a friend
ENDIF
Buy a round of drinks.
```

In this instance, one or other of the blocks will be executed. Then execution will continue with the statements after the ENDIF statement (in this case *buy a round*).

There is yet another extension to the BLOCK IF which allows an ELSEIF statement. Consider the following example:

```
IF (Today == Monday) THEN
   .
ELSEIF (Today == Tuesday) THEN
```

```
   .
ELSEIF (Today == Wednesday) THEN
   .
ELSEIF (Today == Thursday) THEN
   .
ELSEIF (Today == Friday) THEN
   .
ELSEIF (Today == Saturday) THEN
   .
ELSEIF (Today == Sunday) THEN
   .
ELSE
   there has been an error. The variable Today has
   taken on an illegal value.
ENDIF
```

Note that as soon as one of the logical expressions is true, the rest of the test is skipped, and execution continues with the statements after the ENDIF. This implies that a construction like

```
IF(I < 2)THEN
   ...
ELSEIF(I < 1)THEN
   ...
ELSE
   ...
ENDIF
```

is inappropriate. If I is less than 2, the latter condition will never be tested. The ELSE statement has been used here to aid in trapping errors or exceptions. This is recommended practice. A very common error in programming is to assume that the data are in certain well-specified ranges. The program then fails when the data go outside this range. It makes no sense to have a day other than Monday, Tuesday, Wednesday, Thursday, Friday, Saturday or Sunday.

16.1.2 Example 1: Quadratic roots

A quadratic equation is:

$$a\,x^2 + b\,x + c = 0$$

This program is straightforward, with a simple structure. The roots of the quadratic are either real, equal and real, or complex depending on the magnitude of the term B ** 2 – 4 * A * C. The program tests for this term being greater than or less than

zero: it assumes that the only other case is equality to zero (from the mechanics of a computer, floating point equality is rare, but we are safe in this instance):

```
PROGRAM ch1601
IMPLICIT NONE
REAL :: A , B , C , Term , A2 , Root1 , Root2
!
!    a b and c are the coefficients of the terms
!    a*x**2+b*x+c
!    find the roots of the quadratic, root1 and root2
!
   PRINT*,' GIVE THE COEFFICIENTS A, B AND C'
   READ*,A,B,C
   Term = B*B - 4.*A*C
   A2 = A*2.
! if term < 0, roots are complex
! if term = 0, roots are equal
! if term > 0, roots are real and different
   IF(Term < 0.0)THEN
      PRINT*,' ROOTS ARE COMPLEX'
   ELSEIF(Term > 0.0)THEN
      Term = SQRT(Term)
      Root1 = (-B+Term)/A2
      Root2 = (-B-Term)/A2
      PRINT*,' ROOTS ARE ',Root1,' AND ',Root2
   ELSE
      Root1 = -B/A2
      PRINT*,' ROOTS ARE EQUAL, AT ',Root1
   ENDIF
END PROGRAM ch1601
```

16.1.3 Note

Given the understanding you now have about real arithmetic and finite precision will the ELSE block above ever be executed?

16.1.4 Example 2: Date calculation

This next example is also straightforward. It demonstrates that, even if the conditions on the IF statement are involved, the overall structure is easy to determine. The comments and the names given to variables should make the program self-explanatory. Note the use of integer division to identify leap years:

```
PROGRAM ch1602
IMPLICIT NONE
```

```
INTEGER :: Year , N , Month , Day , T
!
! calculates day and month from year and
! day-within-year
! t is an offset to account for leap years.
! Note that the first criteria is division by 4
! but that centuries are only
! leap years if divisible by 400
! not 100 (4 * 25) alone.
!
   PRINT*,' year, followed by day within year'
   READ*,Year,N
!    checking for leap years
   IF ((Year/4)*4 == Year ) THEN
     T=1
     IF ((Year/400)*400 == Year ) THEN
       T=1
     ELSEIF ((Year/100)*100 == Year) THEN
       T=0
     ENDIF
   ELSE
     T=0
   ENDIF
!     accounting for February
   IF(N > (59+T))THEN
     Day=N+2-T
   ELSE
     Day=N
   ENDIF
   Month=(Day+91)*100/3055
   Day=(Day+91)-(Month*3055)/100
   Month=Month-2
   PRINT*,' CALENDAR DATE IS ', Day , Month , Year
END PROGRAM ch1602
```

16.1.5 The CASE statement

The CASE statement provides a very clear and expressive selection mechanism between two or more courses of action. Strictly speaking it could be constructed from the IF THE ELSE IF ENDIF statement, but with considerable loss of clarity. Remember that programs have to be read and understood by both humans and compilers!

16.1.6 Example 3: Simple calculator

```
PROGRAM ch1603
IMPLICIT NONE
!
! Simple case statement example
!

INTEGER :: I,J,K
CHARACTER :: Operator
  DO
     PRINT *,' Type in two integers'
     READ *, I,J
     PRINT *,' Type in operator'
     READ '(A)',Operator
     Calculator : &
     SELECT CASE (Operator)
       CASE ('+') Calculator
          K=I+J
          PRINT *,' Sum of numbers is ',K
       CASE ('-') Calculator
          K=I-J
          PRINT *,' Difference is ',K
       CASE ('/') Calculator
          K=I/J
          PRINT *,' Division is ',K
       CASE ('*') Calculator
       K=I*J
       PRINT *,' Multiplication is ',K
     CASE DEFAULT Calculator
       EXIT
     END SELECT Calculator
  END DO
END PROGRAM ch1603
```

The user is prompted to type in two integers and the operation that they would like carried out on those two integers. The CASE statement then ensures that the appropriate arithmetic operation is carried out. The program terminates when the user types in any character other than +, -, * or /.

The CASE DEFAULT option introduces the EXIT statement. This statement is used in conjunction with the DO statement. When this statement is executed control passes to the statement immediately after the matching END DO statement. In

the example above the program terminates, as there are no executable statements after the END DO.

16.1.7 Example 4: Counting vowels, consonants, etc.

This example is more complex, but again is quite easy to understand. The user types in a line of text and the program produces a summary of the frequency of the characters typed in:

```
PROGRAM ch1604
IMPLICIT NONE
!
! Simple counting of vowels, consonants,
! digits, blanks and the rest
!
INTEGER :: Vowels=0 , Consonants=0, Digits=0
INTEGER :: Blank=0, Other=0, I
CHARACTER :: Letter
CHARACTER (LEN=80) :: Line
  READ '(A)', Line
  DO I=1,80
    Letter=Line(I:I)
! the above extracts one character at position I
    SELECT CASE (Letter)
      CASE ('A','E','I','O','U', &
            'a','e','i','o','u')
        Vowels=Vowels + 1
      CASE ('B','C','D','F','G','H', &
            'J','K','L','M','N','P', &
            'Q','R','S','T','V','W', &
            'X','Y','Z',             &
            'b','c','d','f','g','h', &
            'j','k','l','m','n','p', &
            'q','r','s','t','v','w', &
            'x','y','z')
        Consonants=Consonants + 1
      CASE ('1','2','3','4','5','6','7','8','9','0')
        Digits=Digits + 1
      CASE (' ')
        Blank=Blank + 1
      CASE DEFAULT
        Other=Other+1
    END SELECT
  END DO
```

```
   PRINT *, ' Vowels =   ', Vowels
   PRINT *, ' Consonants =   ', Consonants
   PRINT *, ' Digits = ', Digits
   PRINT *, ' Blanks = ',Blank
   PRINT *, ' Other characters = ', Other
END PROGRAM ch1604
```

16.2 The three forms of the DO statement

You have already been introduced in the chapters on arrays to the iterative form of the DO loop, i.e.,

DO Variable = Start, End, Increment

block of statements

END DO

A complete coverage of this form is given in the three chapters on arrays.

There are two additional forms of the block DO that complete our requirements:

DO WHILE (Logical Expression)

block of statements

ENDDO

and

DO

block of statements

IF (Logical Expression) EXIT

END DO

The first form is often called a WHILE loop as the block of statements executes whilst the logical expression is true, and the second form is often called a REPEAT UNTIL loop as the block of statements executes until the statement is true.

Note that the WHILE block of statements may never be executed, and the REPEAT UNTIL block will always be executed at least once.

16.2.1 Example 5: Sentinel usage

The following example shows a complete program using this construct:

```
PROGRAM ch1605
IMPLICIT NONE
! this program picks up the first occurrence
```

```
! of a number in a list.
! a sentinel is used, and the array is 1 more
! than the max size of the list.
INTEGER , ALLOCATABLE , DIMENSION(:) :: A
INTEGER :: Mark
INTEGER :: I,Howmany
   OPEN (UNIT=1,FILE='DATA')
   PRINT *,' What number are you looking for?'
   READ  *, Mark
   PRINT *,' How many numbers to search?'
   READ  *,Howmany
   ALLOCATE(A(1:Howmany+1))
   READ(UNIT=1,FMT=*) (A(i),I=1,Howmany)
   I=1
   A(Howmany+1)= Mark
   DO WHILE(Mark /= A(I))
      I=I+1
   END DO
   IF(I == (Howmany+1)) THEN
      PRINT*,' ITEM NOT IN LIST'
   ELSE
      PRINT*,' ITEM IS AT POSITION ',I
   ENDIF
END PROGRAM ch1605
```

The *repeat until* construct is written in Fortran as:

```
   DO
   ...
   ...
      IF (Logical Expression) EXIT
   END DO
```

There are problems in most disciplines that require a numerical solution. The two main reasons for this are either that the problem can only be solved numerically or that an analytic solution involves too much work. Solutions to this type of problem often require the use of the *repeat until* construct. The problem will typically require the repetition of a calculation until the answers from successive evaluations differ by some small amount, decided generally by the nature of the problem. A program extract to illustrate this follows:

```
   REAL , PARAMETER :: TOL=1.0E-6
   .
```

```
DO
   ...
   CHANGE=
   ...
   IF (CHANGE <= TOL) EXIT
END DO
```

Here the value of the tolerance is set to 1.0E–6. Note again the use of the EXIT statement. The DO END DO block is terminated and control passes to the statement immediately after the matching END DO.

16.2.2 CYCLE and EXIT

These two statements are used in conjunction with the block DO statement. You have seen examples above of the use of the EXIT statement to terminate the block DO, and pass control to the statement immediately after the corresponding END DO statement.

The CYCLE statement can appear anywhere in a block DO and will immediately pass control to the start of the block DO. Examples of CYCLE and EXIT are given in later chapters.

16.2.3 Example 6: e**x evaluation

The function etox illustrates one use of the *repeat until* construct. The function evaluates e**x. This may be written as

$$1 + x/1! + x^2/2! + x^3/3! \ldots$$

or

$$1+\sum_{n=1}^{\infty} \frac{x^{n-1}}{(n-1)!}\frac{x}{n}$$

Every succeeding term is just the previous term multiplied by *x/n*. At some point the term *x/n* becomes very small, so that it is not sensibly different from zero, and successive terms add little to the value. The function therefore repeats the loop until *x/n* is smaller than the tolerance. The number of evaluations is not known beforehand, since this is dependent on *x*:

```
REAL FUNCTION etox(X)
IMPLICIT NONE
REAL :: Term
REAL , INTENT(IN) :: X
INTEGER :: Nterm
REAL , PARAMETER ::Tol = 1.0E-6
  etox=1.0
```

```
   Term=1.0
   Nterm=0
   DO
      Nterm = Nterm +1
      Term =( X / Nterm) * Term
      etox = etox + Term
      IF(ABS(Term) <= Tol)EXIT
   END DO
END FUNCTION etox

program ch1606
implicit none
real :: etox
real , parameter :: x=1.0
real :: y
   print *,' Fortran intrinsic ',exp(x)
   y=etox(x)
   print *,' User defined etox ',y
end program ch1606
```

The whole program compares the user defined function with the Fortran intrinsic exp function.

16.2.4 Example 7: Wave breaking on an offshore reef

This example is drawn from a situation where a wave breaks on an offshore reef or sand bar, and then reforms in the near-shore zone before breaking again on the coast. It is easier to observe the heights of the reformed waves reaching the coast than those incident to the terrace edge.

Both types of loops are combined in this example. The algorithm employed here finds the zero of a function. Essentially, it finds an interval in which the zero must lie; the evaluations on either side are of different signs. The *while loop* ensures that the evaluations are of different signs, by exploiting the knowledge that the incident wave height must be greater than the reformed wave height (to give the lower bound). The upper bound is found by experiment, making the interval bigger and bigger. Once the interval is found, its mean is used as a new potential bound. The zero must lie on one side or the other; in this fashion, the interval containing the zero becomes smaller and smaller, until it lies within some tolerance. This approach is rather plodding and unexciting, but is suitable for a wide range of problems

Here is the program:

```
PROGRAM Break
IMPLICIT NONE
REAL :: Hi , Hr , Hlow , High , Half , Xl
REAL :: Xh , Xm , D
REAL , PARAMETER :: Tol=1.0E-6
! problem - find hi from expression given
! in function f
! F=A*(1.0-0.8*EXP(-0.6*C/A))-B
! HI IS INCIDENT WAVE HEIGHT          (C)
! HR IS REFORMED WAVE HEIGHT          (B)
! D IS WATER DEPTH AT TERRACE EDGE    (A)
   PRINT*,' Give reformed wave height, and water depth'
   READ*,Hr,d
!
! for Hlow- let Hlow=hr
! for high- let high=Hlow*2.0
!
! check that signs of function results are different
!
   Hlow = Hr
   High = Hlow*2.0
   Xl = F( Hlow, Hr, D)
   Xh = F( High, Hr, D)
!
   DO WHILE ((XL*XH)  >= 0.0)
      HIGH = HIGH*2.0
      XH = F(HIGH,HR,D)
   END DO
!
   DO
      HALF=(HLOW+HIGH)*0.5
      XM=F(HALF,HR,D)
      IF((XL*XM) < 0.0)THEN
         XH=XM
         HIGH=HALF
      ELSE
         XL=XM
         HLOW=HALF
      ENDIF
      IF(ABS(HIGH-HLOW)<= TOL)EXIT
   END DO
   PRINT*,' Incident Wave Height Lies Between'
```

```
   PRINT*,Hlow,' and ',High,' metres'
CONTAINS
REAL FUNCTION F(A,B,C)
IMPLICIT NONE
REAL , INTENT (IN) :: A
REAL , INTENT (IN) :: B
REAL , INTENT (IN) :: C
   F=A*(1.0-0.8*EXP(-0.6*C/A))-B
END FUNCTION F
END PROGRAM Break
```

16.3 Summary

You have been introduced in this chapter to several control structures and these include:

- The *block if*.
- The *if then else if*.
- The *case* construct.
- The block *do* in three forms:
  - The *iterative do* or *do variable=start,end,increment ... end do*.
  - The *while* construct, or *do while ... end do*.
  - The *repeat until* construct, or *do ... if then exit end do*.
- The *cycle* and *exit* statements, which can be used with *do* statement in all three forms:
  - The *do variable = start,end,increment ... end do*.
  - The *while* construct, or *do while ... end do*.
  - The *repeat until* construct, or *do ... if then exit end do.*

These constructs are sufficient for solving a wide class of problems. There are other control statements available in Fortran, especially those inherited from Fortran 66 and Fortran 77, but those covered here are the ones preferred. We will look in Chapter 28 at one more control statement, the so-called GOTO statement, with recommendations as to where its use is appropriate.

16.3.1 Control structure formal syntax

CASE

```
SELECT CASE ( case variable )
   [ CASE case selector
      [executable construct ] ... ] ...
   [ CASE DEFAULT
   [executable construct ]
END SELECT
```

DO

```
DO [ label ]
   [executable construct ] ...
do termination

DO [ label ] [ , ] loop variable = initial value ,
final value , [ increment ]
   [executable construct ] ...
do termination

DO [ label ] [ , ] WHILE (scalar logical expression )
   [executable construct ] ...
do termination
```

IF

```
IF ( scalar logical expression ) THEN
   [executable construct ] ...
[ ELSE IF ( scalar logical expression  THEN
   [executable construct ] ... ] ...]
[ ELSE
      [executable construct ] ...]
END IF
```

16.4 Problems

1. Rewrite the program for the period of a pendulum. The new program should print out the length of the pendulum and period, for pendulum lengths from 0 to 100 cm in steps of 0.5 cm. The program should incorporate a function for the evaluation of the period.

2. Write a program to read an integer that must be positive.

Hint. Use a DO WHILE to make the user re-enter the value.

3. Using functions, do the following:

- Evaluate $n!$ from $n = 0$ to $n = 10$.

- Calculate 76!
- Now calculate (*x****n*)/*n*!, with $x = 13.2$ and $n = 20$.
- Now do it another way.

4. The program BREAK is taken from a real example. In the particular problem, the reformed wave height was 1 metre, and the water depth at the reef edge was 2 metres. What was the incident wave height? Rather than using an absolute value for the tolerance, it might be more realistic to use some value related to the reformed wave height. These heights are unlikely to be reported to better than about 5% accuracy. Wave energy may be taken as proportional to wave height squared for this example. What is the reduction in wave energy as a result of breaking on the reef or bar for this particular case.

5. What is the effect of using INT on negative real numbers? Write a program to demonstrate this.

6. How would you find the nearest integer to a real number? Now do it another way. Write a program to illustrate both methods. Make sure you test it for negative as well as positive values.

7. The function etox has been given in this chapter. The standard Fortran function EXP does the same job. Do they give the same answers? Curiously the Fortran standard does not specify how a *standard* function should be evaluated, or even how accurate it should be.

The physical world has many examples in which processes require that some threshold be overcome before they begin operation: critical mass in nuclear reactions, a given slope to be exceeded before friction is overcome, and so on. Unfortunately, most of these sorts of calculations become rather complex and not really appropriate here. The following problem tries to restrict the range of calculation, whilst illustrating the possibilities of decision making.

8. If a cubic equation is expressed as

$$z^3 + a_2 z^2 + a_1 z + a_0 = 0$$

and we let

$$q = \frac{a_1}{3} - \frac{(a_2 * a_2)}{9}$$

and

$$r = \frac{(a_1 * a_2 - 3 * a_0)}{6} - \frac{(a_2 * a_2 * a_2)}{27}$$

we can determine the nature of the roots as follows:

$q^3 + r^2 > 0$; one real root and a pair of complex
$q^3 + r^2 = 0$; all roots real, and at least two equal
$q^3 + r^2 < 0$; all roots real

Incorporate this into a suitable program, to determine the nature of the roots of a cubic from suitable input.

9. The form of breaking waves on beaches is a continuum, but for convenience we commonly recognise three major types: surging, plunging and spilling. These may be classified empirically by reference to the wave period, T (seconds), the breaker wave height, H_b (metres), and the beach slope, m. These three variables are combined into a single parameter, B, where

$$B = H_b/(gmT^2)$$

g is the gravitational constant (981 cm s^{-2}). If B is less than 0.003, the breakers are surging; if B is greater than 0.068, they are spilling, and between these values, plunging breakers are observed.

(i) On the east coast of New Zealand, the normal pattern is swell waves, with wave heights of 1 to 2 metres and wave periods of 10 to 15 seconds. During storms, the wave period is generally shorter, say 6 to 8 seconds, and the wave heights higher, 3 to 5 metres. The beach slope may be taken as about 0.1. What changes occur in breaker characteristics as a storm builds up?

(ii) Similarly, many beaches have a concave profile. The lower beach generally has a very low slope, say less than 1 degree (m = 0.018), but towards the high-tide mark, the slope increases dramatically, to say 10 degrees or more (m = 0.18). What changes in wave type will be observed as the tide comes in?

16.5 Bibliography

Dahl O.J., Dijkstra E.W., Hoare C.A.R., *Structured Programming*, Academic Press, 1972.

- This is the original text, and a must. The quote at the start of the chapter by Dijkstra summarises beautifully our limitations when programming and the discipline we must have to master programming successfully.

Knuth D.E., *Structured Programming with GOTO Statements,* in Current Trends in Programming Methodology, Volume 1, Prentice-Hall, 1977.

- The chapter by Knuth provides a very succinct coverage of the arguments for the adoption of structured programming, and dispels many of the myths concerning the use of the GOTO statement. Highly recommended.

17

Characters

"These metaphysics of magicians,
And necromantic books are heavenly;
Lines, circles, letters and characters."

Christopher Marlowe, *The Tragical History of Doctor Faustus*

Aims

The aims of this chapter are:

- To extend the ideas about characters introduced in earlier chapters.
- To demonstrate that this enables us to solve a whole new range of problems in a satisfactory way.

17 Characters

For each type in a programming language there are the following concepts:

- Values are drawn from a finite domain.
- There are a restricted number of operations defined for each type.

For the numeric types we have already met, integers and reals:

- The values are either drawn from the domain of integer numbers or the domain of real numbers.
- The valid operations are addition, subtraction, multiplication, division and exponentiation.

For the character data type the basic unit is an individual character — any character which is available on your keyboard normally. To ensure portability we should restrict ourselves to the Fortran character set, that is:

- the alphabetic characters A through Z, the digits or numeric characters 0 through 9, and the underscore character _

which may be used in variable names, and the complete Fortran character set is given in section 7.6 in Chapter 7.

This provides us with 58 printing characters and omits many commonly used characters, e.g., lower case letters. However, if one does work with this set then one can ensure that programs are portable.

As the most common current internal representation for the character data type uses 8 bits this should provide access to 256 (2^8) characters. However, there is little agreement over the encoding of these 256 possible characters, and the best you can normally assume is access to the ASCII character set, which is given in Appendix B. One of the problems at the end of this chapter looks at determining what characters one has available.

The only operations defined are concatenation (joining character strings together) and comparison.

We will look into the area of character sets in more depth later in this chapter.

We can declare our character variables:

```
CHARACTER :: A, String, Line
```

Note that there is no default typing of the character variable (unlike integer and real data types), and we can use any convenient name within the normal Fortran conventions. In the declaration above, each character variable would have been

permitted to store one character. This is limiting, and, to allow character strings which are several units long, we have to add one item of information:

```
CHARACTER (10) :: A
CHARACTER (16) :: String
CHARACTER (80) :: Line
```

This indicates that A holds 10 characters, STRING holds 16, and LINE holds 80. If all the character variables in a single declaration contain the same number of characters, we can abbreviate the declaration to

```
CHARACTER(80) :: LIST, STRING, LINE
```

But we cannot mix both forms in the one declaration. We can now assign data to these variables, as follows:

```
   A='FIRST ONE '
   STRING='A LONGER ONE     '
   LINE='THE QUICK BROWN FOX JUMPS OVER THE LAZY DOG'
```

The delimiter apostrophe (') or quotation mark (“) is needed to indicate that this is a character string (otherwise the assignments would have looked like invalid variable names).

17.1 Character input

In an earlier chapter we saw how we could use the READ * and PRINT * statements to do both numeric and character input and output or I/O. When we use this form of the statement we have to include any characters we type within delimiters (either the apostrophe ' or the quotation mark “). This is a little restricting and there is a slightly more complex form of the READ statement that allows one to just type the string on its own. The following two programs illustrate the differences:

```
PROGRAM ch1701
!
! Simple character i/o
!
CHARACTER (80) :: Line
   READ *, Line
   PRINT *, Line
END PROGRAM ch1701
```

This form requires enclosing the string with delimiters. Consider the next form:

```
PROGRAM ch1702
!
! Simple character i/o
!
CHARACTER (80) :: Line
   READ '(A)' , Line
   PRINT *,Line
END PROGRAM ch1702
```

With this form one can just type the string in and input terminates with the carriage return key. The additional syntax involves '(A)' where '(A)' is a character edit descriptor. The simple examples we have used so far have used implied format specifiers and edit descriptors. For each data type we have one or more edit descriptors to choose from. For the character data type only the A edit descriptor is available.

17.2 Character operators

The first manipulator is a new operator — the concatenation operator //. With this operator we can join two character variables to form a third, as in

```
CHARACTER (5) :: FIRST, SECOND
CHARACTER (10) :: THIRD
FIRST='THREE'
SECOND='BLIND'
...
THIRD=FIRST//SECOND
.
THIRD=FIRST//'MICE'
```

Where there is a discrepancy between the created length of the concatenated string and the declared lengths of the character strings, truncation will occur. For example,

```
THIRD=FIRST//' BLIND MICE'
```

will only append the first five characters of the string ' BLIND MICE' i.e., ' BLIN', and THIRD will therefore contain 'THREE BLIN'.

What would happen if we assigned a character variable of length 'n' a string which was shorter than n? For example,

```
CHARACTER (4) :: C2
C2='AB'
```

The remaining two characters are considered to be blank, that is, it is equivalent to saying

```
C2='AB  '
```

However, while the strings 'AB' and 'AB ' are equivalent, 'AB' and ' AB' are not. In the jargon, the character strings are always *left justified,* and the *unset* characters are trailing blanks.

If we concatenate strings which have 'trailing blanks', the blanks, or spaces, are considered to be legitimate characters, and the concatenation begins after the end of the first string. Thus

```
CHARACTER (4) :: C2,C3
CHARACTER (8) :: JJ
C2='A'
C3='MAN'
JJ=C2//C3
PRINT*, 'THE CONCATENATION OF ',C2,' AND ',C3,' IS'
PRINT*,JJ
```

would appear as

THE CONCATENATION OF A AND MAN GIVES

A MAN

at the terminal.

Sometimes we need to be able to extract parts of character variables — substrings. The actual notation for doing this is a little strange at first, but it is very powerful. To extract a substring we must reference two items:

- The position in the string at which the substring begins.

and

- The position at which it ends.

e.g.,

```
STRING='SHARE AND ENJOY'
```

17.3 Character substrings

We may extract parts of this string:

```
BIT=STRING(3:5)
```

would place the characters 'ARE' into the variable BIT. This may be manipulated further:

```
BIT1=STRING(2:4)//STRING(9:9)
BIT2=STRING(5:5) // &
STRING(3:3)//STRING(1:1)//STRING(15:15)
```

Note that to extract a *single* character we reference its beginning position and its end (i.e., repeat the same position), so that

```
STRING(3:3)
```

gives the single character 'A'. The substring reference can cut out either one of the two numerical arguments. If the first is omitted, the characters up to and including the reference are selected, so that

```
SUB=STRING(:5)
```

would result in SUB containing the characters 'SHARE'. When the second argument is omitted, the characters from the reference are selected, so that

```
SUB=STRING(11:)
```

would place the characters 'ENJOY' in the variable SUB. In these examples it would also be necessary to declare STRING, SUB, BIT, BIT1 and BIT2 to be of CHARACTER type, of some appropriate length.

Character variables may also form arrays:

```
CHARACTER (10) , DIMENSION(20) :: A
```

sets up a character array of twenty elements, where each element contains ten characters. In order to extract substrings from these array elements, we need to know where the array reference and the substring reference are placed. The array reference comes first, so that

```
DO I=1,20
   FIRST=A(I)(1:1)
ENDO
```

places the first character of each element of the array into the variable FIRST. The syntax is therefore 'position in array, followed by position within string'.

Any argument can be replaced by a variable:

```
STRING(I:J)
```

This offers interesting possibilities, since we can, for example, strip blanks out of a string:

```
PROGRAM ch1703
IMPLICIT NONE
  CHARACTER(80) :: String, Strip
  INTEGER :: IPOS,I,Length=80
  IPOS=0
  PRINT *,' Type in a string'
  READ '(A)',String
  DO I=1,Length
    IF(String(I:I) /= ' ') THEN
      IPOS=IPOS+1
      Strip(IPOS:IPOS)=String(I:I)
    ENDIF
  END DO
  PRINT*,String
  PRINT*,Strip
END PROGRAM ch1703
```

17.4 Character functions

There are special functions available for use with character variables: INDEX will give the starting position of a string within another string. If, for example, we were looking for all occurrences of the string 'Geology' in a file, we could construct something like:

```
PROGRAM ch1704
IMPLICIT NONE
CHARACTER (80) :: Line
INTEGER :: I
  DO
    READ '(A)', Line
    I=INDEX(Line,'Geology')
    IF (I /= 0) THEN
      PRINT *, ' String Geology found at position ',I
      PRINT *, ' in line ', Line
      EXIT
    ENDIF
  ENDDO
END PROGRAM ch1704
```

There are two things to note about this program. Firstly the INDEX function will only report the first occurrence of the string in the line; any later occurrences in

any particular line will go unnoticed, unless you account for them in some way. Secondly, if the string does not occur, the result of the INDEX function is zero, and given the infinite loop (DO ENDDO) the program will crash at run time with an end of file error message. This isn't good programming practice.

LEN provides the length of a character string. This function is not immediately useful, since you really ought to know how many characters there are in the string. However, as later examples will show, there are some cases where it can be useful. Remember that trailing blanks do count as part of the character string, and contribute to the length.

The following example illustrates the use of both LEN and LEN_TRIM:

```
PROGRAM ch1705
IMPLICIT NONE
CHARACTER (LEN=20) :: Name
INTEGER :: Name_Length
   PRINT *,' Type in your name'
   READ  '(A)',Name
!
! show LEN first
!
   Name_length=LEN(Name)
   PRINT *,' Name length is ',Name_length
   PRINT *,' ',Name(1:Name_length),'<-end is here'
   Name_length=LEN_TRIM(Name)
   PRINT *,' Name length is ',Name_length
   PRINT *,' ',Name(1:Name_Length),'<-end is here'
END PROGRAM ch1705
```

17.5 Collating sequence

The next group of functions need to be considered together. They revolve around the concept of a collating sequence. In other words, each character used in Fortran is ordered as a list and given a corresponding *weight*. No two weights are equal. Although Fortran has only 58 defined characters, the machine you use will generally have more; 95 printing characters is a typical minimum number. On this type of machine the weights would vary from 0 to 94. There is a defined collating sequence, the ASCII sequence, which is likely to be the default. The parts of the collating sequence which are of most interest are fairly standard throughout all collating sequences.

In general, we are interested in the numerals (0–9), the alphabetics (A–Z) and a few odds and ends like the arithmetic operators (+ – / *), some punctuation (. and ,) and perhaps the prime ('). As you might expect, 0–9 carry successively higher

weights (though not the weights 0 to 9), as do A to Z. The other odds and ends are a little more problematic, but we can find out the weights through the function ICHAR. This function takes a single character as argument and returns an integer value. The ASCII weights for the alphanumerics are as follows:

0–9	48–57
A–Z	65–90

One of the exercises is to determine the weights for other characters. The reverse of this procedure is to determine the character from its weighting, which can be achieved through the function CHAR. CHAR takes an integer argument and returns a single character. Using the ASCII collating sequence, the alphabet would be generated from

```
DO   I=65,90
   PRINT*,CHAR(I)
ENDDO
```

This idea of a weighting can then be used in four other functions:

Function	Action
LLE	Lexically less than or equal to
LGE	Lexically greater than or equal to
LGT	Lexically greater than
LLT	Lexically less than

In the sequence we have seen before, A is lexically less than B, i.e., its weight is less. Clearly, we can use ICHAR and get the same result. For example,

```
IF(LGT('A','B')) THEN
```

is equivalent to

```
IF(ICHAR('A') > ICHAR('B')) THEN
```

but these functions can take character string arguments of any length. They are not restricted to single characters.

These functions provide very powerful tools for the manipulation of characters, and open up wide areas of nonnumerical computing through Fortran. Text format-

ting and word processing applications may now be tackled (conveniently ignoring the fact that lower-case characters may not be available).

There are many problems that require the use of character variables. These range from the ability to provide simple titles on reports, or graphical output, to the provision of a natural language interface to one of your programs, i.e., the provision of an English-like command language. *Software Tools* by Kernighan and Plauger contains many interesting uses of characters in Fortran.

17.6 Summary

Characters represent a different data type to any other in Fortran, and as a consequence there is a restricted range of operations which may be carried out on them.

A character variable has a length which must be assigned in a CHARACTER declaration statement.

Character strings are delimited by apostrophes (') or quotation marks (“). Within a character string, the blank is a significant character.

Character strings may be joined together (concatenated) with the // operator.

Substrings occurring within character strings may be also be manipulated. There are a number of functions especially for use with characters:

- ACHAR
- ADJUSTL
- ADJUSTR
- CHAR
- IACHAR
- INDEX
- LEN
- LEN_TRIM
- LLE
- LGE
- LGT
- LLT
- REPEAT
- SCAN

- TRIM
- VERIFY

17.7 Problems

1. Suggest some circumstances where PRIME="" might be useful. What other alternative is there and why do you think we use that instead?

2. Write a program to write out the weights for the Fortran character set. Modify this program to print out the weights of the complete implementation defined character set for your version of Fortran 90. Is it ASCII? If not, how does it differ?

3. Use the INDEX function in order to find the location of all the strings 'IS' in the following data:

IF A PROGRAMMER IS FOUND TO BE INDISPENSABLE, THE BEST THING TO DO IS TO GET RID OF HIM AS QUICKLY AS POSSIBLE.

4. Find the 'middle' character in the following strings. Do you include blanks as characters? What about punctuation?

PRACTICE IS THE BEST OF ALL INSTRUCTORS. EXPERIENCE IS A DEAR TEACHER, BUT FOOLS WILL LEARN AT NO OTHER.

5. In English, the order of occurrence of the letters, from most frequent to least is

E, T, A, O, N, R, I, S, H, D, L, F, C, M, U, G, Y, P, W, B, V, K, X, J, Q, Z

Use this information to examine the two files given in Appendix D (one is a translation of the other) to see if this is true for these two extracts of text. The second text is in medieval Latin (c. 1320). Note that a fair amount of compression has been achieved by expressing the passage in Latin rather than modern English. Does this provide a possible model for information compression?

6. A very common cypher is the substitution cypher, where, for example, every letter A is replaced by (say) an M, every B is replaced by (say) a Y, and so on. These encyphered messages can be broken by reference to the frequency of occurrence of the letters (given in the previous question).

Since we know that (in English) E is the most commonly occurring letter, we can assume that the most commonly occurring letter in the encyphered message represents an E; we then repeat the process for the next most common and so on. Of course, these correspondences may not be exact, since the message may not be long enough to develop the frequencies fully.

However, it may provide sufficient information to break the cypher.

The file given in Appendix E contains an encoded message. Break it. Clue — *Pg Fybdujuvef jo Tdjfodf,* Jorge Luis Borges.

18

Complex

“Make it as simple as possible, but no simpler.”

Albert Einstein

“'Can you do addition?' the White Queen asked. 'What's one and one and one and one and one and one and one and one and one and one?' 'I don't know' said Alice. 'I lost count.' 'She can't do addition,' the Red Queen interrupted.”

Lewis Carroll, *Through the Looking Glass and What Alice Found There.*

Aims

The aims of this chapter are:

- To introduce the last predefined numeric data type in Fortran.
- To illustrate with examples how to use this type.

18 Complex

This variable type reflects an extension of the real data type available in Fortran — the COMPLEX data type, where we can store and manipulate complex variables. Problems that require this data type are restricted to certain branches of mathematics, physics and engineering. Complex numbers are defined as having a *real* and *imaginary* part, i.e.,

$$a = x + \mathrm{i}y$$

where i is the square root of –1.

They are not supported in many programming languages as a base type which makes Fortran the language of first choice for many people.

To use this variable type we have to write the number as two parts, the real and imaginary elements of the number, for example,

```
COMPLEX :: U
   U=(1.0,2.0)
```

represents the complex number 1 + i2. Note that the complex number is enclosed in brackets. We can do arithmetic on variables like this, and most of the intrinsic functions such as LOG, SIN, COS, etc., accept a complex data type as argument.

All the usual rules about mixing different variable types, like reals and integers, also apply to complex. Complex numbers are read in and written out in a similar way to real numbers, but with the provision that, for each single complex value, two format descriptors must be given. You may use either E or F formats (or indeed, mix them), as long as there are enough of them. Although you use brackets around the pairs of numbers in a program, these must not appear in any input, nor will they appear on the output.

Fortran has a number of functions which help to clarify the intent of *mixed mode* expressions. The functions REAL, CMPLX and INT can be used to 'force' any variable to real, complex or integer type.

There are a number of intrinsic functions to enable complex calculations to be performed. The program segment below uses some of them:

```
COMPLEX:: Z, Z1,Z2,Z3,ZBAR
REAL :: X,Y,X1,Y1,X2,Y2,X3,Y3,ZMOD
   Z1 = CMPLX (1.0, 2.0)      !  1 + i 2
   Z2 = CMPLX(X2, Y2)         ! X2 + i Y2
   Z3 = CMPLX (X3, Y3)        ! X3 + i Y3
   Z  = Z1*Z2 / Z3
```

```
   X   = REAL(Z)                ! real part of Z
   Y   = AIMAG (Z)              ! imaginary part of Z
   ZMOD = ABS(Z)                ! modulus of Z
   ZBAR = CONJG(Z)              ! complex conjugate of Z
```

18.1 Example

The second order differential equation:

$$\frac{d^2 y}{d t^2} + 2\frac{dy}{dt} + y = x(t)$$

could describe the behaviour of an electrical system, where *x(t)* is the input voltage and *y*(*t*) is the output voltage and *dy/dt* is the current. The complex ratio

$$\frac{y(w)}{x(w)} = 1 \,/\, (-w^2 + 2\ j\ w + 1)$$

is called the frequency response of the system because it describes the relationship between input and output for sinusoidal excitation at a frequency of *w* and where *j* is $\sqrt{-1}$. The following program segment reads in a value of *w* and evaluates the frequency response for this value of *w* together with its polar form (magnitude and phase):

```
PROGRAM ch1801
IMPLICIT NONE
!
! Program to calculate frequency response of a system
! for a given Omega
! and its polar form (magnitude and phase).
!
REAL :: Omega ,Real_part , Imag_part , Magnitude, Phase
COMPLEX:: Frequency_response
!
! Input frequency Omega
!
   PRINT *, 'Input frequency'
   READ *,Omega
!
   Frequency_response = 1.0 / &
      CMPLX( - Omega * Omega + 1.0 , 2.0 * Omega)
   Real_part = REAL(Frequency_response)
   Imag_part = AIMAG(Frequency_response)
!
```

```
! Calculate polar coordinates (magnitude and phase)
!
   Magnitude = ABS(Frequency_response)
   Phase = ATAN2 (Imag_part, Real_part)
!
   PRINT *, ' At frequency ',Omega
   PRINT *, 'Response = ', Real_part,' + I ',Imag_part
   PRINT *, 'in Polar form'
   PRINT *, ' Magnitude = ', Magnitude
   PRINT *, ' Phase = ', Phase
END PROGRAM ch1801
```

18.2 Complex and kind type

The standard requires that there be a minimum of two kind types for real numbers and this is also true of the complex data type. Chapter 8 must be consulted for a full coverage of real kind types. We would therefore use something like the following to select a complex kind type other than the default:

```
INTEGER , PARAMETER ::
Long_Complex=SELECTED_REAL_KIND(15,307)
COMPLEX (Long_Complex) :: Z
```

Chapter 24 includes a good example of how to use modules to define and use precision throughout a program and subprogram units.

18.3 Summary

COMPLEX is used to store and manipulate complex numbers: those with a real and an imaginary part.

There are standard functions which allow conversion between the numerical data types — CMPLX, REAL and INT.

18.4 Problems

1. The program used in Chapter 15 which calculated the roots of a quadratic had to abandon the calculation if the roots were complex. You should now be able to remedy this, remembering that it is necessary to declare any complex variables. Instead of raising the expression to the power 0.5 in order to take its square root, use the function SQRT. If you manage this to your satisfaction, try your skills on the roots of a cubic (see the problems in Chapter 15).

19

Logical

"A messenger yes/no semaphore
her black/white keys in/out whirl of morse
hoopooe signals salvation deviously."

Nathaniel Tarn, *The Laurel Tree*

Aims

The aims of this chapter are:

- To examine the last predefined type available in Fortran: logical.
- To introduce the concepts necessary to use logical expressions effectively, namely:
  - Logical variables.
  - Logical operators.
  - The hierarchy of operations.
  - Truth tables.

19 Logical

Often we have situations where we need ON/OFF, TRUE/FALSE or YES/NO switches, and in such circumstances we can use LOGICAL type variables, e.g.,

```
LOGICAL :: FLAG
```

Logicals may take only two possible values, as shown in the following:

```
FLAG=.TRUE.
```

or

```
FLAG=.FALSE.
```

Note the full stops, which are essential. With a little thought you can see why they are needed. You will already have met some of the ideas associated with logical variables from IF statements:

```
IF(A == B) THEN
   .
ELSE
   .
ENDIF
```

The logical expression (A == B) returns a value *true* or *false,* which then determines the route to be followed; if the quantity is true, then we execute the next statement, else we take the other route.

Similarly, the following example is also legitimate:

```
LOGICAL :: ANSWER
   ANSWER=.TRUE.
   ...
   IF (ANSWER) THEN
      ...
   ELSE
      ...
   ENDIF
```

Again the expression IF (ANSWER) is evaluated; here the variable ANSWER has been set to .TRUE., and therefore the statements following the THEN are executed. Clearly, conventional arithmetic is inappropriate with logicals. What does 2 times true mean? (very true?). There are a number of special operators for logicals:

.NOT. which negates a logical value (i.e., changes *true* to *false* or vice versa).

.AND. logical intersection.

.OR. logical union.

To illustrate the use of these operators, consider the following program extract:

```
LOGICAL :: A,B,C
   A=.TRUE.
   B=.NOT.A
!                    (B now has the value 'false')
   C=A.OR.B
!                    (C has the value 'true')
   C=A.AND.B
!                    (C now has the value 'false')
```

To gauge the effect of these operators on logicals, we can consult a truth table:

X1	X2	.NOT.X1	X1.AND.X2	X1.OR.X2
true	true	false	true	true
true	false	false	false	true
false	true	true	false	true
false	false	true	false	false

As with arithmetic operators, there is an order of precedence associated with the logical operators:

.AND. is carried out before

.OR. and .NOT.

In dealing with logicals, the operations are carried out within a given level, from left to right. Any expressions in brackets would be dealt with first. The logical operators are a lower order of precedence than the arithmetic operators, i.e., they are carried out later. A more complete operator hierarchy is therefore:

- Expressions within brackets.
- Exponentiation.
- Multiplication/division.

- Addition/subtraction.
- Relational logical (= =, >, <, >=, <= /=).
- .AND.
- .OR. and .NOT.

Although you can build up complicated expressions with mixtures of operators, these are often difficult to comprehend, and it is generally more straightforward to break '*big*' expressions down into smaller ones whose purpose is more readily appreciated.

Historically, logicals have not been in evidence extensively in Fortran programs, although clearly there are occasions on which they are of considerable use. Their use often aids significantly in making programs more modular and comprehensible. They can be used to make a complex section of code involving several choices much more transparent by the use of one logical function, with an appropriate name. Logicals may be used to control output; e.g.,

```
LOGICAL :: DEBUG
   ...
   DEBUG=.TRUE.
   ...
   IF(DEBUG)THEN
      ...
      PRINT *,'LOTS OF PRINTOUT'
      ...
   ENDIF
```

ensures that, while debugging a program you have more output. Then, when the program is *correct*, run with DEBUG=.FALSE.

Note that Fortran does try to protect you while you use logical variables. You cannot do the following:

```
LOGICAL :: UP, DOWN
   UP=DOWN+.FALSE.
```

or

```
LOGICAL :: A2
   REAL DIMENSION(10):: OMEGA
   .
   A2=OMEGA(3)
```

The compiler will note that this is an error, and will not permit you to run the program. This is an example of *strong typing*, since only a limited number of predetermined operations are permitted. The real, integer and complex variable types are much more weakly typed (which helps lead to the confusion inherent in mixing variable types in arithmetic assignments).

19.1 I/O

Since logicals may take only the values .TRUE. and .FALSE., the possibilities in reading and writing logical values are clearly limited. The L edit descriptor or format allows logicals to be input and output. On input, if the first nonblank characters are either T or .T, the logical value .TRUE. is stored in the corresponding list item; if the first nonblank characters are F or .F, then .FALSE. is stored. (Note therefore that reading, say, TED and FAHR in an L4 format would be acceptable.) If the first nonblank character is not F, T, .F or .T, then an error message will be generated. On output, the value T or F is written out, right justified, with blanks (if appropriate). Thus,

```
LOGICAL :: FLAG
   FLAG=.TRUE.
   PRINT 100, FLAG, .NOT.FLAG
   100 FORMAT(2L3)
```

would produce

```
T   F
```

at the terminal.

Assigning a logical variable to anything other than a .TRUE. or .FALSE. value in your program will result in errors. The 'shorthand' forms of .T, .F, F and T are not acceptable in the program.

19.2 Summary

Another type of data — logical — is also recognised. A LOGICAL variable may take one of two values — *true* or *false*.

- There are special operators for manipulating logicals:
  - .NOT.
  - .AND.
  - .OR.
- Logical operators have a lower order of precedence than any others.

19.3 Problems

1. Why are the full stops needed in a statement like A = .TRUE.?

2. Generate a truth table like the one given in this chapter.

3. Write a program which will read in numerical data from the terminal, but will *flag* any data which is negative, and will also turn these negative values into positive ones.

20

User Defined Types

"Russell's theory of types leads to certain complexities in the foundations of mathematics... Its interesting features for our purposes are that types are used to prevent certain erroneous expressions from being used in logical and mathematical formulae; and that a check against violation of type constraints can be made purely by scanning the text, without any knowledge of the value which a particular symbol might happen to have."

C.A.R. Hoare, *Structured Programming*

Aims

The aim of this chapter is to introduce the concepts and ideas involved in using the facilities offered in Fortran 90 for the construction and use of user defined types:

- The way in which we define our own types.
- The way in which we declare variables to be of a user defined type.
- The way in which we manipulate variables of our own types.
- The way in which we can nest types within types.

The examples are simple and are designed to highlight the syntax. More complex and realistic examples of the use of user defined data types are to be found in later chapters.

20 User Defined Types

In the coverage so far we have used the intrinsic types provided by Fortran. The only data structuring technique available has been to construct arrays of these intrinsic types. Whilst this enables us to solve a reasonable variety of problems, it is inadequate for many purposes. In this chapter we look at the facilities offered by Fortran for the construction of our own types and how we manipulate data of these new, user defined types.

With the ability to define our own types we can now construct aggregate data types that have components of a variety of base types. These are often given the name records in books on data structures. In mathematics the term cartesian product is often used, and this is the terminology adopted by Hoare. We will stick to the term records, as it is the one that is most commonly used in computing and texts on programming.

There are two stages in the process of creating and using our own data types: we must first define the type, and then create variables of this type.

20.1 Example 1: Dates

```
PROGRAM ch2001
IMPLICIT NONE
TYPE Date
   INTEGER :: Day=1
   INTEGER :: Month=1
   INTEGER :: Year=2000
END TYPE Date
TYPE (Date) :: D
   PRINT *,D%Day, D%Month, D%Year
   PRINT *,' Type in the date, day, month, year'
   READ *,D%Day, D%Month, D%Year
   PRINT *,D%Day, D%Month, D%Year
END PROGRAM ch2001
```

This complete program illustrates both the definition and use of the type. It also shows how you can define initial values within the type definition.

20.2 Type definition

The type *Date* is defined to have three component parts, comprising a *day*, a *month* and a *year*, all of integer type. The syntax of a type construction comprises:

TYPE Typename
  Data Type :: Component_name
  etc
END TYPE Typename

Reference can then be made to this new type by the use of a single word, *Date*, and we have a very powerful example of the use of abstraction.

20.3 Variable definition

This is done by

```
TYPE (Typename) :: Variablename
```

and we then define a variable *D* to be of this new type. The next thing we do is have a READ * statement that prompts the user to type in three integer values, and the data are then echoed straight back to the user. We use the notation `Variablename%Component_Name` to refer to each component of the new data type.

20.4 Example 2: Address lists

```
PROGRAM ch2002
IMPLICIT NONE
TYPE Address
   CHARACTER (LEN=40) :: Name
   CHARACTER (LEN=60) :: Street
   CHARACTER (LEN=60) :: District
   CHARACTER (LEN=60) :: City
   CHARACTER (LEN=8)  :: Post_Code
END TYPE Address
INTEGER , PARAMETER :: N_of_Address=78
TYPE (Address) , DIMENSION(N_of_Address):: Addr
INTEGER :: I
   OPEN(UNIT=1,FILE="ADDRESS.DAT")
   DO I=1,N_of_Address
      READ(UNIT=1,FMT='(A40)') Addr(I)%Name
      READ(UNIT=1,FMT='(A60)') Addr(I)%Street
      READ(UNIT=1,FMT='(A60)') Addr(I)%District
      READ(UNIT=1,FMT='(A60)') Addr(I)%City
      READ(UNIT=1,FMT='(A8)') Addr(I)%Post_Code
   END DO
   DO I=1,N_of_Address
      PRINT *,Addr(I)%Name
```

```
      PRINT *,Addr(I)%Street
      PRINT *,Addr(I)%District
      PRINT *,Addr(I)%City
      PRINT *,Addr(I)%Post_Code
   END DO
END PROGRAM ch2002
```

In this example we define a type Address which has components that one would expect for a person's address. We then define an array Addr of this type. Thus we are now creating arrays of our own user defined types. We index into the array in the way we would expect from our experience with integer, real and character arrays. The complete example is rather trivial in a sense in that the program merely reads from one file and prints the file out to the screen. However, it highlights many of the important ideas of the definition and use of user defined types.

20.5 Example 3: Nested user defined types

The following example builds on the two data types already introduced. Here we construct nested user defined data types based on them and construct a new data type containing them both plus additional information:

```
PROGRAM ch2003
IMPLICIT NONE
TYPE Address
   CHARACTER (LEN=60)   :: Street
   CHARACTER (LEN=60)   :: District
   CHARACTER (LEN=60)   :: City
   CHARACTER (LEN=8 )   :: Post_Code
END TYPE Address
TYPE Date_Of_Birth
   INTEGER :: Day
   INTEGER :: Month
   INTEGER :: Year
END TYPE Date_Of_Birth
TYPE Personal
   CHARACTER (LEN=20)    :: First_Name
   CHARACTER (LEN=20)    :: Other_Names
   CHARACTER (LEN=40)    :: Surname
   TYPE (Date_Of_Birth) :: DOB
   CHARACTER (LEN=1)     :: Sex
   TYPE (Address)         :: Addr
END TYPE Personal
INTEGER , PARAMETER :: N_People=2
```

```
TYPE (Personal) , DIMENSION(N_People) :: P
INTEGER :: I
   OPEN(UNIT=1,FILE='PERSON.DAT')
   DO I=1,N_People
      READ(1,FMT=10) P(I)%First_Name,&
                     P(I)%Other_Names,&
                     P(I)%Surname,&
                     P(I)%DOB%Day,&
                     P(I)%DOB%Month,&
                     P(I)%DOB%Year,&
                     P(I)%Sex,&
                     P(I)%Addr%Street,&
                     P(I)%Addr%District,&
                     P(I)%Addr%City,&
      P(I)%Addr%Post_Code
      10 FORMAT(  A20,/,&
                  A20,/,&
                  A40,/,&
                  I2,1X,I2,1X,I4,/,&
                  A1,/,&
                  A60,/,&
                  A60,/,&
                  A60,/,&
                  A8)
   END DO
   DO I=1,N_People
      WRITE(*,FMT=20)   P(I)%First_Name,&
                        P(I)%Other_Names,&
                        P(I)%Surname,&
                        P(I)%DOB%Day,&
                        P(I)%DOB%Month,&
                        P(I)%DOB%Year,&
                        P(I)%Sex,&
                        P(I)%Addr%Street,&
                        P(I)%Addr%District,&
                        P(I)%Addr%City,&
                        P(I)%Addr%Post_Code
      20 FORMAT(        A20,A20,A40,/,&
                        I2,1X,I2,1X,I4,/,&
                        A1,/,&
                        A60,/,&
                        A60,/,&
```

```
                              A60,/,&
                              A8)
   END DO
END PROGRAM ch2003
```

Here we have a date of birth data type (`Date_Of_Birth`) based on the `Date` data type from the first example, plus a slightly modified address data type, incorporated into a new data type comprising personal details. Note the way in which we reference the component parts of this new, aggregate data type.

20.6 Problems

1. Modify the last example to include a more elegant printed name. The current example will pad with blanks the first name, other names and surname and span 80 characters on one line, which looks rather ugly.

Add a new variable name which will comprise all three subcomponents and write out this new variable, instead of the three subcomponents.

20.7 Bibliography

Dahl O.J., Dijkstra E.W., Hoare C.A.R., *Structured Programming*, Academic Press, 1972.

- This is one of the earliest and best introductions to data structures and structured programming. The whole book hangs together very well, and the section on data structures is a must for serious programmers.

Vowels R.A., *Algorithms and Data Structures in F and Fortran*, Unicomp, 1989.

- One of the few books looking at algorithms and data structures using Fortran.

Wirth N., *Algorithms + Data Structures = Programs*, Prentice-Hall, 1976.

Wirth N., *Algorithms + Data Structures*, Prentice-Hall, 1986.

- The first is in Pascal, and the second in Modula 2.

Wood D., *Paradigms and Programming in Pascal*, Computer Science Press, 1984.

- Contains a number of examples of the use of recursion in problem solving. Also provides a number of useful case studies in problem solving.

21

An Introduction to Pointers

"The question naturally arises whether the analogy can be extended to a data structure corresponding to recursive procedures. A value of such a type would be permitted to contain more than one component that belongs to the same type as itself; in the same way that a recursive procedure can call itself recursively from more than one place in its own body."

C.A.R. Hoare, *Structured Programming*

Aim

The primary aim of the chapter is to introduce some of the key concepts of pointers in Fortran.

21 An Introduction to Pointers

All of the data types introduced so far, with the exception of the allocatable array, have been static. Even with the allocatable array a size has to be set at some stage during program execution. The facilities provided in Fortran by the concept of a pointer combined with those offered by a user defined type enable us to address a completely new problem area, previously extremely difficult to solve in Fortran. There are many problems where one genuinely does not know what requirements there are on the size of a data structure. Linked lists allow sparse matrix problems to be soved with minimal storage requirements, two-dimensional spatial problems can be addressed with quad-trees and three-dimensional spatial problems can be addressed with oct-trees. Many problems also have an irregular nature, and pointer arrays address this problem.

First we need to cover some of the technical aspects of pointers. A pointer is a variable that has the POINTER attribute. A pointer is associated with a target by allocation or pointer assignment. A pointer becomes associated as follows:

- The pointer is allocated as the result of the successful execution of an ALLOCATE statement referencing the pointer

or

- The pointer is pointer-assigned to a target that is associated or is specified with the TARGET attribute and, if allocatable, is currently allocated.

A pointer shall neither be referenced nor defined until it is associated. A pointer is disassociated following execution of a DEALLOCATE or NULLIFY statement, following pointer association with a disassociated pointer, or initially through pointer initialisation.

A pointer may have a pointer association status of associated, disassociated, or undefined. Its association status may change during execution of a program. Unless a pointer is initialised (explicitly or by default), it has an initial association status of undefined. A pointer may be initialised to have an association status of disassociated.

Let us look at some examples to clarify these points.

21.1 Some basic pointer concepts

With the introduction of pointers as a data type into Fortran we also have the introduction of a new assignment statement — the pointer assignment statement. Consider the following example:

```
PROGRAM C2101
   INTEGER , POINTER :: A,B
```

```
    INTEGER , TARGET :: C
    INTEGER :: D
    C = 1
    A => C
    C = 2
    B => C
    D = A + B
    PRINT *,A,B,C,D
END PROGRAM C2101
```

The first declaration defines A and B to be variables, with the POINTER attribute. This means we can use A and B to refer or point to integer values. Note that in this case no space is set aside for the pointer variables A and B. A and B should not be referenced in this state.

The second declaration defines C to be an integer, with the TARGET attribute, i.e., we can use pointers to refer or point to the value of the variable C.

The last declaration defines D to be an ordinary integer variable.

In the case of the last two declarations space is set aside to hold two integers.

Let us now look at the various executable statements in the program, one at a time:

C = 1	This is an example of the normal assignment statement with which we are already familiar. We use the variable name C in our program and whenever we use that name we get the *value* of the variable C.
A => C	This is an example of a pointer assignment statement. This means that both A and C now refer to the same value, in this case 1. A becomes associated with the target C. A can now be referenced.
C = 2	Conventional assignment statement, and C now has the value 2.
B = > C	Second example of pointer assignment. B now points to the value that C has, in this case 2. B becomes associated with the target C. B can now be referenced.
D = A + B	Simple arithmetic assignment statement. The value that A points to is added to the value that B points to and the result is assigned to D.

The last statement prints out the values of A, B, C and D.

The output is

```
 2  2  2  4
```

21.2 The ASSOCIATED intrinsic function

The ASSOCIATED intrinsic returns the association status of a pointer variable. Consider the following example:

```
PROGRAM C2102
INTEGER , POINTER :: A,B
INTEGER , TARGET :: C
INTEGER :: D
   PRINT *,ASSOCIATED(A)
   PRINT *,ASSOCIATED(B)
   C = 1
   A => C
   C = 2
   B => C
   D = A + B
   PRINT *,A,B,C,D
   PRINT *,ASSOCIATED(A)
   PRINT *,ASSOCIATED(B)
END PROGRAM C2102
```

The output from running this program with a number of compilers is shown below.

21.2.1 CVF 6.6C

```
 F
 F
              2               2               2
4
 T
 T
```

21.2.2 Intel, Windows, 8.1

```
F
F
2  2  2  4
T
T
```

21.2.3 Lahey, Windows 5.70f

```
F
F
2  2  2  4
T
```

```
T
```

21.2.4 NAG, Windows, 4.2

```
 T
 T
 2  2  2  4
 T
 T
```

21.2.5 Salford 4.6.0

```
    T
    T
                2               2               2
4
    T
    T
```

We have some differences, and the actual answer as to why is rather subtle. The standard says that the ASSOCIATED function must not be called with a pointer whose status is undefined. So in this program we have declared the pointers A and B but their initial status is undefined. So in a sense all of the above could be regarded as correct, as the program breaks the standard!

The next example is a simple variant.

21.3 Referencing A and B before assignment

Consider the following example:

```
PROGRAM C2103
INTEGER , POINTER :: A,B
INTEGER , TARGET :: C
INTEGER :: D
   PRINT *,ASSOCIATED(A)
   PRINT *,ASSOCIATED(B)
   PRINT *,A
   PRINT *,B
   C = 1
   A => C
   C = 2
   B => C
   D = A + B
   PRINT *,A,B,C,D
   PRINT *,ASSOCIATED(A)
```

```
   PRINT *,ASSOCIATED(B)
END PROGRAM C2103
```

Here we are actually referencing the pointer, even though its status is undefined. Most compilers generate a run time error with this example. However, the error message tends to be a little cryptic. Some sample outputs with the default compilation options follow

21.3.1 CVF

```
 F
 F
forrtl: severe (157): Program Exception - access
violation
Image                  PC          Routine
Line          Source
ch2003cvf.exe        00401098   C2003
7   ch2003.f90
ch2003cvf.exe        004266A9   Unknown
Unknown   Unknown
ch2003cvf.exe        0041D9E4   Unknown
Unknown   Unknown
kernel32.dll         7C816D4F   Unknown
Unknown   Unknown
```

21.3.2 Intel, Windows 8.1

```
 F
 F
forrtl: severe (157): Program Exception - access
violation
Image                  PC          Routine
Line          Source
ch2003intel.exe     0040106E   Unknown
Unknown   Unknown
ch2003intel.exe     0043DE2D   Unknown
Unknown   Unknown
ch2003intel.exe     00430D60   Unknown
Unknown   Unknown
kernel32.dll         7C816D4F   Unknown
Unknown   Unknown
```

21.3.3 Lahey, Windows 5.70f

```
F
F
jwe0019i-u The program was terminated abnormally with
Exception Code EXCEPTION_ACCESS_VIOLATION.
 Error occurs at or near line 6 of _MAIN__
error summary (Fortran)
error number   error level   error count
  jwe0019i           u             1
total error count = 1
```

21.3.4 NAG, Windows 4.2

```
 T
 T
Segmentation fault (core dumped)
```

21.3.5 Salford 4.6.0

```
    T
    T
   -2130131837
               1
               2              2              2
4
    T
    T
```

Some of the compilers give a clue with a line number. The Salford output is interesting as the program actually ran to completion. Try and find compiler options that will provide better diagnostic error messages with your compiler.

21.4 The NULL intrinsic

Fortran 95 introduced the NULL intrinsic. The three previous examples are to a degree examples of Fortran 90 style programming:

```
PROGRAM C2104
INTEGER , POINTER :: A=>NULL(),B=>NULL()
INTEGER , TARGET :: C
INTEGER :: D
   PRINT *,ASSOCIATED(A)
   PRINT *,ASSOCIATED(B)
   C = 1
   A => C
```

```
   C = 2
   B => C
   D = A + B
   PRINT *,A,B,C,D
   PRINT *,ASSOCIATED(A)
   PRINT *,ASSOCIATED(B)
END PROGRAM C2104
```

All compilers tested gave the same correct result. The recommendation is therefore to always use the NULL intrinsic to provide pointer variables with a known value of disassociated, rather than undefined.

21.5 Assignment via =

Consider the following two examples:

```
PROGRAM C2105
INTEGER , POINTER :: A=>NULL(),B=>NULL()
INTEGER , TARGET :: C
INTEGER :: D
   C = 1
   A = 21
   C = 2
   B => C
   D = A + B
   PRINT *,A,B,C,D
END PROGRAM C2105
```

and

```
PROGRAM C2106
INTEGER , POINTER :: A=>NULL(),B=>NULL()
INTEGER , TARGET :: C
INTEGER :: D
   C = 1
   A => C
   C = 2
   B = A
   D = A + B
   PRINT *,A,B,C,D
END PROGRAM C2106
```

Both of these will compile but both will generate run time errors. In the first program the problems lies with the statement

```
   A = 21
```

and in the second case the problem lies with the statement

```
   B = A
```

Below are the corrected versions of the programs

```
PROGRAM C2107
INTEGER , POINTER :: A=>NULL(),B=>NULL()
INTEGER , TARGET :: C
INTEGER :: D
   ALLOCATE(A)
   C = 1
   A = 21
   C = 2
   B => C
   D = A + B
   PRINT *,A,B,C,D
END PROGRAM C2107
```

and

```
PROGRAM C2108
INTEGER , POINTER :: A=>NULL(),B=>NULL()
INTEGER , TARGET :: C
INTEGER :: D
   ALLOCATE(B)
   C = 1
   A => C
   C = 2
   B = A
   D = A + B
   PRINT *,A,B,C,D
END PROGRAM C2108
```

Our recommendation when using pointers is to nullify them when declaring them and to explicitly allocate them before using them when assigning a value via normal assignment.

21.6 Singly linked list

Conceptually a singly linked lists consists of a sequence of boxes with compartments. In the simplest case the first compartment holds a data item and the second contains directions to the next box.

We can construct a data structure in Fortran to work with a singly linked list by combining the concept of a record from the previous chapter with the new concept of a pointer. A complete program to do this is given below:

```
PROGRAM C2109
TYPE Link
   CHARACTER :: C
   TYPE (Link) , POINTER    :: Next
END TYPE Link
TYPE (Link) , POINTER :: Root , Current
INTEGER :: IO_Stat_Number=0
   ALLOCATE(Root)
   READ (UNIT = *, FMT = '(A)' , ADVANCE = 'NO' , &
     IOSTAT = IO_Stat_Number) Root%C
   IF (IO_Stat_Number == -1) THEN
      NULLIFY(Root%Next)
   ELSE
      ALLOCATE(Root%Next)
   ENDIF
   Current => Root
   DO WHILE (ASSOCIATED(Current%Next))
      Current => Current%Next
      READ (UNIT=*,FMT='(A)',ADVANCE='NO', &
      IOSTAT=IO_Stat_Number) Current%C
      IF (IO_Stat_Number == -1) THEN
         NULLIFY(Current%Next)
      ELSE
         ALLOCATE(Current%Next)
      ENDIF
   END DO
   Current => Root
   DO WHILE (ASSOCIATED(Current%Next))
      PRINT * , Current%C
      Current => Current%Next
   END DO
END PROGRAM C2109
```

The behaviour of this program is system specific. You will have to look at your compiler documentation regarding the IO_Stat_Number. The first thing of interest is the type definition for the singly linked list. We have

```
TYPE Link
   CHARACTER :: C
   TYPE (Link) , POINTER :: Next
END TYPE Link
```

and we call the new type `Link`. It comprises two component parts: the first holds a character `C`, and the second holds a pointer called `Next` to allow us to refer to another instance of type `Link`. Remember we are interested in joining together several boxes or `Links`.

The next item of interest is the variable definition. Here we define two variables `Root` and `Current` to be pointers that point to items of type `Link`. In Fortran when we define a variable to be a pointer we also have to define what it is allowed to point to. This is a very useful restriction on pointers, and helps make using them more secure.

The first executable statement

```
ALLOCATE(Root)
```

requests that the variable `Root` be allocated memory. At this time the contents of both the character component and the pointer component are undefined.

The next statement reads a character from the keyboard. We are using a number of additional features of the READ statement, including

```
ADVANCE='NO'
IOSTAT=IO_Stat_Number
```

and the two options combine to provide the ability to read an arbitrary amount of text from the user per line, and terminate only when end of file is encountered as the only input on a line, typically by typing CTRL Z. Note that the numbers returned by the IOSTAT option are implementation specific. A small program would have to be written to test the values returned for each platform.

If an end of file is reached then the pointer `Root%Next` is nullified using the NULLIFY statement. This gives the pointer a status of disassociated, and this is a convenient way of saying that it doesn't point to anything valid.

If the end of file is not detected then the next link in the chain is created.

The statement

```
Current => Root
```

means that both `Current` and `Root` point to the same physical memory location, and this holds a character data item and a pointer. We must do this as we have to know where the start of the list is. This is now our responsibility, not the compilers. Without this statement we are not able to do anything with the list except fill it up — hardly very useful.

The WHILE loop is then repeated until end of file is reached. If the user had typed an end of file immediately then `Current%Next` would not be ASSOCIATED, and the WHILE loop would be skipped.

This loop allocates memory and moves down the chain of boxes one character at a time filling in the links between the boxes as we go. We then have

```
Current => Root
```

and this now means that we are back at the start of the list, and in a position to traverse the list and print out each character in the list.

There is thus the concept with the pointer variable Current of it providing us with a window into memory where the complete linked list is held, and we look at one part of the list at a time.

Both WHILE loops use the intrinsic function ASSOCIATED to check the association status of a pointer.

It is recommended that this program be typed in, compiled and executed. It is surprisingly difficult to believe that it will actually read in a completely arbitrary number of characters from the user. Seeing is believing.

21.7 Reading in an arbitrary quantity of numeric data

In this example we will look at using a singly linked list to read in an arbitrary quantity of data and then allocating an array to copy it to for normal numeric calculations at run time:

```
PROGRAM C2110

TYPE Link
   REAL :: N
   TYPE (Link) , POINTER    :: Next
END TYPE Link

TYPE (Link) , POINTER :: Root, Current
```

```
INTEGER :: I=0
integer :: error=0
INTEGER :: IO_Stat_Number=0
integer :: blank_lines=0

real , allocatable , dimension(:) :: x

   ALLOCATE(Root)
   READ (UNIT = *, FMT = *, IOSTAT = IO_Stat_Number)
Root%N
   IF (IO_Stat_Number > 0) THEN
      error=error+1
   else if (io_stat_number == -1) then
      NULLIFY(Root%Next)
   else if (io_stat_number == -2) then
      blank_lines=blank_lines+1
   ELSE
      i=i+1
      ALLOCATE(Root%Next)
   ENDIF

   Current => Root

   DO WHILE (ASSOCIATED(Current%Next))

      Current => Current%Next

      READ (UNIT=*,FMT=*, IOSTAT=IO_Stat_Number)
Current%N

      IF (IO_Stat_Number > 0) THEN
         error=error+1
      else if (io_stat_number == -1) then
         NULLIFY(current%Next)
      else if (io_stat_number == -2) then
         blank_lines=blank_lines+1
      ELSE
         i=i+1
         ALLOCATE(current%Next)
      ENDIF
```

```
   END DO

   print *,i,' items read'
   print *,blank_lines,' blank lines'
   print *,error,' items in error'

   allocate(x(1:i))
   i=1
   Current => Root

   DO WHILE (ASSOCIATED(Current%Next))
      x(i)=current%n
      i=i+1
      PRINT * , Current%N
      Current => Current%Next
   END DO

   print *,x

END PROGRAM C2110
```

Below is a variant on this using the NAG compiler. Note the use of a module and meaningful names for the status of the read:

```
PROGRAM C2111

use f90_iostat

TYPE Link
   REAL :: N
   TYPE (Link) , POINTER    :: Next
END TYPE Link

TYPE (Link) , POINTER :: Root, Current

INTEGER :: I=0
INTEGER :: IO_Stat_Number=0

   ALLOCATE(Root)
   READ (UNIT = *, FMT = *, IOSTAT = IO_Stat_Number)
Root%N
   if (io_stat_number == ioerr_eof) then
      NULLIFY(Root%Next)
```

```
   ELSE if(io_stat_number == ioerr_ok) then
      i=i+1
      ALLOCATE(Root%Next)
   ENDIF

   Current => Root

   DO WHILE (ASSOCIATED(Current%Next))

      Current => Current%Next

      READ (UNIT=*,FMT=*, IOSTAT=IO_Stat_Number)
Current%N

      if (io_stat_number == ioerr_eof) then
         NULLIFY(current%Next)
      ELSE if(io_stat_number == ioerr_ok) then
         i=i+1
         ALLOCATE(current%Next)
      ENDIF

   END DO

   print *,i,' items read'

   Current => Root

   DO WHILE (ASSOCIATED(Current%Next))
      PRINT * , Current%N
      Current => Current%Next
   END DO

END PROGRAM C2111
```

21.8 Arrays of pointers

Arrays in Fortran are rectangular, even when allocatable. So if you wish to set up a lower triangular matrix that uses minimal memory you have to use arrays of pointers. The following examples show how to do this.

```
PROGRAM C2112
IMPLICIT NONE
TYPE Ragged
```

```
   REAL , DIMENSION(:) , POINTER :: Ragged_row
END TYPE
INTEGER :: i
INTEGER , PARAMETER :: n=3
TYPE (Ragged) , DIMENSION(1:n) :: Lower_Diag
   DO i=1,n
      ALLOCATE(Lower_Diag(i)%Ragged_Row(1:i))
      PRINT *,' Type in the values for row ' , i
      READ *,Lower_Diag(I)%Ragged_Row(1:i)
   END DO
   DO i=1,n
      PRINT *,Lower_Diag(i)%Ragged_Row(1:i)
   END DO
END PROGRAM C2112
```

The type Ragged has a component that is a pointer to an array. Within the first DO loop we allocate a row at a time and each time we go around the loop the array allocated increases in size.

21.9 Arrays of pointers and variable sized data sets — 1

In this example we use a parameter statement to set up the number of stations:

```
PROGRAM C2113
IMPLICIT NONE
TYPE Ragged
  REAL , DIMENSION(:) , POINTER :: rainfall
END TYPE
INTEGER :: i
INTEGER , PARAMETER :: nr=5
INTEGER , DIMENSION (1:nr) :: nc
TYPE (ragged) ,  DIMENSION(1:nr) :: station
  DO i=1,nr
     PRINT *,' enter the number of data values' &
      ' for station ',i
     READ *,nc(i)
     ALLOCATE(station(i)%rainfall(1:nc(i)))
     PRINT *,' Type in the values for station ' , i
     READ *,station(i)%rainfall(1:nc(i))
  END DO
  DO i=1,nr
     PRINT *,station(i)%rainfall(1:nc(i))
  END DO
```

```
END PROGRAM C2013
```

We read in the dimension or number of values for each station at run time, and allocate the space at run time.

21.10 Arrays of pointers and variable sized data sets — 2

In this example the number of stations is read in at run time:

```
PROGRAM C2114
IMPLICIT NONE
TYPE Ragged
  REAL , DIMENSION(:) , POINTER :: rainfall
END TYPE
INTEGER :: i
INTEGER :: nr
iNTEGER , ALLOCATABLE , DIMENSION (:) :: nc
TYPE (ragged) , ALLOCATABLE ,  DIMENSION(:) :: station
  PRINT *,' enter number of stations'
  READ *,nr
  ALLOCATE(station(1:nr))
  ALLOCATE(nc(1:nr))
  DO I=1,Nr
    PRINT *,' enter the number of data values ' &
     ' for station ',i
    READ *,nc(i)
    ALLOCATE(station(i)%rainfall(1:nc(i)))
    PRINT *,' Type in the values for station ' , I
    READ *,station(i)%rainfall(1:nc(i))
  END DO
  DO i=1,nr
    PRINT *,station(i)%rainfall(1:nc(i))
  END DO
END PROGRAM C2114
```

In this example both the number of stations and the dimension for each station is read in at run time and allocated accordingly.

21.11 Memory leak examples

Dynamic memory brings greater versatility but requires greater responsibility. Consider the following example:

```
PROGRAM C2115
IMPLICIT NONE
INTEGER :: Allocate_status=0
REAL , DIMENSION(:) , POINTER :: X
REAL , DIMENSION(1:10) , TARGET :: Y
INTEGER , PARAMETER :: SIZE=10000000
INTEGER :: I
   ALLOCATE(X(1:SIZE),STAT=Allocate_status)
   IF (allocate_status > 0) THEN
      PRINT *,' Allocate failed. Program ends.'
      STOP
   ENDIF
! initialise the memory that x points to
    DO I=1,SIZE
       X(I)=I
    END DO
! print out the first 10 values
    DO I=1,10
       PRINT *,X(I)
    END DO
! initialise the array y
    DO I=1,10
       Y(I)=I*I
    END DO
! print out y
    DO I=1,10
       PRINT *,Y(I)
    END DO
! x now points to y
    X=>Y
! print out what x now points to
    DO I=1,10
       PRINT *,X(I)
    END DO
! what has happened to the memory that x
! used to point to?
END PROGRAM C2115
```

The next is a simple variant on the above:

```
PROGRAM C2116
IMPLICIT NONE
INTEGER :: Allocate_status=0
```

```
REAL , DIMENSION(:) , POINTER :: X
REAL , DIMENSION(1:10) , TARGET :: Y
INTEGER , PARAMETER :: SIZE=10000000
INTEGER :: I
  DO
    ALLOCATE(X(1:SIZE),STAT=Allocate_status)
    IF (allocate_status > 0) THEN
      PRINT *,' Allocate failed. Program ends.'
      STOP
    ENDIF

! initialise the memory that x points to
    DO I=1,SIZE
      X(I)=I
    END DO
! print out the first 10 values
    DO I=1,10
      PRINT *,X(I)
    END DO
! initialise the array y
    DO I=1,10
      Y(I)=I*I
    END DO
! print out y
    DO I=1,10
      PRINT *,Y(I)
    END DO
! x now points to y
    X=>Y
! print out what x now points to
    DO I=1,10
      PRINT *,X(I)
    END DO
! what has happened to the memory that x
! used to point to?
  end do
END PROGRAM C2116
```

Before running this example we recommend starting up a memory monitoring program.

Under Microsoft Windows XP Professional holding [CTRL] + [ALT] + [DEL] will bring up the Windows Task Manager. Choose the [Performance] tab to get a

screen which will show CPU usage, PF Usage, CPU Usage History and Page File Usage History. You will also get details of Physical and Kernel memory usage.

Under Linux type

```
top
```

in a terminal window.

In these examples we also see the recommended form of the ALLOCATE statement when working with arrays. This enables us to test if the allocation has worked and take action accordingly. A positive value indicates an allocation error, zero indicates OK.

21.12 Nonstandard pointer examples

Some Fortran compilers provide a LOC intrinsic. The description from the CVF on line documentation follows:

result = LOC (x)
x (Input) is a variable, an array or a record field reference, a procedure, or a constant; it can be of any data type. It must not be the name of an internal procedure or statement function. If it is a pointer, it must be defined and associated with a target.

This returns the address of the variable passed. Below are four examples that show some of what is happening behind the scenes when using pointer variables. We have also included some sample output:

```
PROGRAM C2117
INTEGER , POINTER :: A,B
INTEGER , TARGET :: C
INTEGER :: D
   PRINT *,LOC(a)
   PRINT *,LOC(b)
   PRINT *,LOC(c)
   PRINT *,LOC(d)
   C = 1
   A => C
   C = 2
   B => C
   D = A + B
   PRINT *,A,B,C,D
   PRINT *,LOC(a)
   PRINT *,LOC(b)
   PRINT *,LOC(c)
```

```
   PRINT *,LOC(d)
END PROGRAM C2117
```

CVF Output:

```
              0
              0
      4424172
      4424168
              2             2             2
4
      4424172
      4424172
      4424172
      4424168
```

Lahey Output:

```
0
0
4456968
4456972
2  2  2  4
4456968
4456968
4456968
4456972
```

The value zero is often used to signify a special memory value in computing. After the pointer assignments it is clear that all three variables point to the same value:

```
PROGRAM C2018
INTEGER , POINTER :: A=>NULL(),B=>NULL()
INTEGER , TARGET :: C
INTEGER :: D
   PRINT *,LOC(a)
   PRINT *,LOC(b)
   PRINT *,LOC(c)
   PRINT *,LOC(d)
   C = 1
   A => C
   C = 2
   B => C
   D = A + B
```

```
   PRINT *,A,B,C,D
   PRINT *,LOC(a)
   PRINT *,LOC(b)
   PRINT *,LOC(c)
   print *,loc(d)
END PROGRAM C2018
```

CVF Output:

```
              0
              0
      4424168
      4424164
              2              2              2
4
      4424168
      4424168
      4424168
      4424164
```

Lahey Output:

```
0
0
4456968
4456972
2  2  2  4
4456968
4456968
4456968
4456972
```

We have again the use of zero as the special memory value:

```
PROGRAM C2119
INTEGER , POINTER :: A=>NULL(),B=>NULL()
INTEGER , TARGET :: C
INTEGER :: D
   PRINT *,LOC(a)
   PRINT *,LOC(b)
   ALLOCATE(a)
   ALLOCATE(b)
   PRINT *,LOC(a)
   PRINT *,LOC(b)
```

```
   PRINT *,LOC(c)
   PRINT *,LOC(d)
   C = 1
   A => C
   C = 2
   B => C
   D = A + B
   PRINT *,A,B,C,D
   PRINT *,LOC(a)
   PRINT *,LOC(b)
   PRINT *,LOC(c)
   PRINT *,LOC(d)
END PROGRAM C2119
```

CVF Output:

```
              0
              0
      3292304
      3292328
      4424152
      4424148
              2              2              2
4
      4424152
      4424152
      4424152
      4424148
```

Lahey Output:

```
0
0
8915968
8916160
4457148
4457152
2  2  2  4
4457148
4457148
4457148
4457152
```

In this example we actually use the ALLOCATE statement to set aside space for the pointers. What is interesting in this example is that the original space set aside becomes lost after the pointer assignments. This indicates a small memory leak:

```
PROGRAM C2020
INTEGER , POINTER :: A=>NULL(),B=>NULL()
INTEGER , TARGET :: C
INTEGER :: D
   PRINT *,LOC(a)
   PRINT *,LOC(b)
   ALLOCATE(a)
   ALLOCATE(b)
   PRINT *,LOC(a)
   PRINT *,LOC(b)
   PRINT *,LOC(c)
   PRINT *,LOC(d)
   C = 1
   A = 21
   C = 2
   B = A
   D = A + B
   PRINT *,A,B,C,D
   PRINT *,LOC(a)
   PRINT *,LOC(b)
   PRINT *,LOC(c)
   PRINT *,LOC(d)
END PROGRAM C2020
```

CVF Output:

```
              0
              0
      3292304
      3292328
      4424152
      4424148
            21            21             2            42
      3292304
      3292328
      4424152
      4424148
```

Lahey Output:

```
0
0
8915968
8916160
4457152
4457156
21  21  2  42
8915968
8916160
4457152
4457156
```

In this case the addresses for A and B remain the same as for a normal assignment, not a pointer assignment.

21.13 Problems

1. Compile and run all of the example programs in this chapter with your compiler and examine the output.

2. There are a number of ways of handling exceptions with the READ statement, and we have used the IOSTAT option in this chapter. Consider the following program:

```
PROGRAM C2102p
INTEGER :: IO_Stat_Number=0
INTEGER :: I
   DO
      READ (UNIT=* , FMT=10 , ADVANCE='NO' &
      , IOSTAT=IO_Stat_Number) I
      10 FORMAT(I3)

! 0   = no error
!       no end of file (eof)
!       no end of record (eor)
! -   = eor or eof
! +   = an error occurred

      PRINT *,' iostat=',IO_Stat_Number
      PRINT *,I
   END DO
END PROGRAM C2102p
```

This program is a simple test of the IOSTAT values of whatever system you work on. Try typing in a variety of values including minimally:

- A valid three-digit number + [RETURN] key.
- A three-digit number with an embedded blank, e.g., 1 2 + [RETURN] key.
- [RETURN] key only.
- [CTRL] + Z.
- Any other non-numeric character on the keyboard.
- 100200300 + [RETURN] key.
- [CTRL] + C

This will enable us to program exactly the kind of behaviour we want from I/O and can be used as a code segment for other programs.

22

Introduction to Subroutines

"A man should keep his brain attic stacked with all the furniture he is likely to use, and the rest he can put away in the lumber room of his library, where he can get at it if he wants."

Sir Arthur Conan Doyle, *Five Orange Pips*

Aims

The aims of this chapter are:

- To consider some of the reasons for the inclusion of subroutines in a programming language.
- To introduce with a concrete example some of the concepts and ideas involved with the definition and use of subroutines.
    - The INTERFACE statement and interface blocks.
    - Arguments or parameters.
    - The INTENT attribute for parameters.
    - The CALL statement.
    - Scope of variables.
    - Local variables and the SAVE attribute.
    - The use of parameters to report on the status of the action carried out in the subroutine.

22 Introduction to Subroutines

In the earlier chapter on functions we introduced two types of function

- Intrinsic functions — which are part of the language.
- User defined functions — by which we extend the language.

We now introduce subroutines which collectively with functions are given the name procedures. Procedures provide a very powerful extension to the language by:

- Providing us with the ability to break problems down into simpler more easily solvable subproblems.
- Allowing us to concentrate on one aspect of a problem at a time.
- Avoiding duplication of code.
- Hiding away messy code so that a main program is a sequence of calls to procedures.
- Providing us with the ability to put together collections of procedures that solve commonly occurring subproblems, often given the name libraries, and generally compiled.
- Allowing us to call procedures from libraries written, tested and documented by experts in a particular field. There is no point in reinventing the wheel!

There are a number of concepts required for the successful use of subroutines and we met some of them in Chapter 15 when we looked at user defined functions. We will extend the ideas introduced there of parameters and introduce the additional concept of an interface block. The ideas are best explained with a concrete example.

Note that we use the terms parameters and arguments interchangeably.

22.1 Example 1

This example is one we met earlier that solves a quadratic equation, i.e., solves $a\,x^{\,2} + b\,x + c = 0$

The program to do this originally was just one program. In the example below we break that problem down into smaller parts and make each part a subroutine. The components are:

- Main program or driving routine.
- Interaction with user to get the coefficients of the equation.

- Solution of the quadratic.

Let us look now at how we do this with the use of subroutines:

```
PROGRAM ch2201
IMPLICIT NONE
! Simple example of the use of a main program and two
! subroutines. One interacts with the user and the
! second solves a quadratic equation,
! based on the user input.

REAL :: P, Q, R, Root1, Root2
INTEGER :: IFail=0
LOGICAL :: OK=.TRUE.
   CALL Interact(P,Q,R,OK)
   IF (OK) THEN
      CALL Solve(P,Q,R,Root1,Root2,IFail)
      IF (IFail == 1) THEN
         PRINT *,' Complex roots,
         PRINT *,' calculation abandoned'
      ELSE
         PRINT *,' Roots are  ',Root1,'  ',Root2
      ENDIF
   ELSE
      PRINT*,' Error in data input program ends'
   ENDIF
END PROGRAM ch2201

SUBROUTINE Interact(A,B,C,OK)
   IMPLICIT NONE
   REAL , INTENT(OUT) :: A
   REAL , INTENT(OUT) :: B
   REAL , INTENT(OUT) :: C
   LOGICAL , INTENT(OUT) :: OK
   INTEGER :: IO_Status=0
   PRINT*,' Type in the coefficients A, B AND C'
   READ(UNIT=*,FMT=*,IOSTAT=IO_Status)A,B,C
   IF (IO_Status == 0) THEN
      OK=.TRUE.
   ELSE
      OK=.FALSE.
   ENDIF
END SUBROUTINE Interact
```

```
SUBROUTINE Solve(E,F,G,Root1,Root2,IFail)
   IMPLICIT NONE
   REAL , INTENT(IN) :: E
   REAL , INTENT(IN) :: F
   REAL , INTENT(IN) :: G
   REAL , INTENT(OUT) :: Root1
   REAL , INTENT(OUT) :: Root2
   INTEGER , INTENT(INOUT) :: IFail
! Local variables
   REAL :: Term
   REAL :: A2
   Term = F*F - 4.*E*G
   A2 = E*2.0
! if term < 0, roots are complex
   IF(Term < 0.0)THEN
      IFail=1
   ELSE
      Term = SQRT(Term)
      Root1 = (-F+Term)/A2
      Root2 = (-F-Term)/A2
   ENDIF
END SUBROUTINE Solve
```

22.1.1 Defining a subroutine

A subroutine is defined as

SUBROUTINE subroutine_name(optional list of dummy arguments)

IMPLICIT NONE

dummy argument type definitions with INTENT

...

END SUBROUTINE subroutine_name

and from the earlier example we have the subroutine

```
SUBROUTINE Interact(A,B,C,OK)
   IMPLICIT NONE
   REAL, INTENT(OUT)::A,B,C
   LOGICAL, INTENT(OUT)::OK


END SUBROUTINE Interact
```

22.1.2 Referencing a subroutine

To reference a subroutine you use the CALL statement:

CALL subroutine_name(optional list of actual arguments)

and from the earlier example the call to subroutine `Interact` was of the form:

```
CALL Interact(P,Q,R,OK)
```

When a subroutine returns to the calling program unit control is passed to the statement following the CALL statement.

22.1.3 Dummy arguments or parameters and actual arguments

Procedures and their calling program units communicate through their arguments. We often use the terms parameter and arguments interchangeably throughout this text. The SUBROUTINE statement normally contains a list of dummy arguments, separated by commas and enclosed in brackets. The dummy arguments have a type associated with them; for example, in subroutine Solve X is of type REAL, but no space is put aside for this in memory. When the subroutine is referenced e.g., CALL Solve(P,Q,R,Root1,Root2,Ifail), then the dummy argument *points* to the actual argument P, which is a variable in the calling program unit. The dummy argument and the actual argument must be of the same type — in this case REAL.

22.1.4 Intent

It is recommended that dummy arguments have an INTENT attribute. In the earlier example subroutine `Solve` has a dummy argument E with INTENT(IN), which means that when the subroutine is referenced or called it is expecting E to have a value, but its value cannot be changed inside the subroutine. This acts as an extra security measure besides making the program easier to understand. For each parameter it may have one of three attributes:

- INTENT(IN), where the parameter already has a value and cannot be altered in the called routine.
- INTENT(OUT), where the parameter does not have a value, and is given one in the called routine.
- INTENT(INOUT), where the parameter already has a value and this is changed in the called routine.

22.1.5 Local variables

We saw with functions that variables could be essentially local to the function and unavailable elsewhere. The concept of local variables also applies to subroutines. In the example above Term and A2 are both local variables to the subroutine `Solve`.

22.1.6 Local variables and the SAVE attribute

Local variables are usually created when a procedure is called and their value lost when execution returns to the calling program unit. To make sure that a local variable retains its values between calls to a subprogram the SAVE attribute can be used on a type statement; e.g.,

```
INTEGER , SAVE :: I
```

means that when this statement appears in a subprogram the value of the local variable I is saved between calls.

22.1.7 Scope of variables

In most cases variables are only available within the program unit that defines them. The introduction of argument lists to functions and subroutines immediately opens up the possibility of data within one program unit becoming available in one or more other program units.

In the main program we declare the variables P, Q, R, Root1, Root2, IFail and OK.

Subroutine `Interact` has no variables locally declared. It works on the arguments A, B, C and OK; which map onto P, Q, R and OK from the main program, i.e., it works with those variables.

Subroutine `Solve` has two locally defined variables, Term and A2. It works with the variables E, F, G, Root1, Root2 and IFail, which map onto P, Q, R, Root1, Root2 and IFail from the main program.

22.1.8 Status of the action carried out in the subroutine

It is also useful to use parameters that carry information regarding the status of the action carried out by the subroutine. With the subroutine `Interact` we use a logical variable OK to report on the status of the interaction with the user. In the subroutine `Solve` we use the status of the integer variable Ifail to report on the status of the solution of the equation.

22.2 Example 2

Consider the following example:

```
program ch2202
implicit none
real :: a,b,c
  a = 1000.0
  b =   20.0
  call divide(a,b,c)
  print *,c
```

```
end program ch2202

subroutine divide(a,b,c)
implicit none
integer , intent(in) :: a
integer , intent(in) :: b
integer , intent(out):: c
  c=a/b
end subroutine divide
```

There is a fundamental problem here. In the main program the variables A, B and C are declared to be of type real. In the subroutine DIVIDE they are integer.

If the main program and subroutine are in one file when compiled then the compiler has the oportunity of catching this mismatch. The Nag f95 compiler release 4.2 and the Salford FTN95 compiler release 4.6.0 both diagnose this error and will not compile the program. The following compilers compiled and executed the code generating the following answers:

CVF 6.6C:	1.4012985E-45
Intel 9.0	1.4012985E-45
Lahey 5.7	1.40129846E-45

Fortran 90 introduced a number of language features to help in this area:

- Interface blocks.
- Contained procedures.
- Modules.

We will look at the first two in this chapter and at modules later on.

22.3 Example 3 — Quadratic example with interface blocks

This is the first example with the addition of interface blocks:

```
PROGRAM ch2203
IMPLICIT NONE
! Simple example of the use of a main program and two
! subroutines. One interacts with the user and the
! second solves a quadratic equation,
! based on the user input.
INTERFACE

  SUBROUTINE Interact(A,B,C,OK)
```

```
      IMPLICIT NONE
      REAL , INTENT(OUT) :: A
      REAL , INTENT(OUT) :: B
      REAL , INTENT(OUT) :: C
      LOGICAL , INTENT(OUT) :: OK
   END SUBROUTINE Interact

   SUBROUTINE Solve(E,F,G,Root1,Root2,IFail)
      IMPLICIT NONE
      REAL , INTENT(IN) :: E
      REAL , INTENT(IN) :: F
      REAL , INTENT(IN) :: G
      REAL , INTENT(OUT) :: Root1
      REAL , INTENT(OUT) :: Root2
      INTEGER , INTENT(INOUT) :: IFail
   END SUBROUTINE Solve

END INTERFACE

REAL :: P, Q, R, Root1, Root2
INTEGER :: IFail=0
LOGICAL :: OK=.TRUE.
   CALL Interact(P,Q,R,OK)
   IF (OK) THEN
      CALL Solve(P,Q,R,Root1,Root2,IFail)
      IF (IFail == 1) THEN
         PRINT *,' Complex roots, calculation abandoned'
      ELSE
         PRINT *,' Roots are  ',Root1,'  ',Root2
      ENDIF
   ELSE
      PRINT*,' Error in data input program ends'
   ENDIF
END PROGRAM ch2203

SUBROUTINE Interact(A,B,C,OK)
   IMPLICIT NONE
   REAL , INTENT(OUT) :: A
   REAL , INTENT(OUT) :: B
   REAL , INTENT(OUT) :: C
   LOGICAL , INTENT(OUT) :: OK
   INTEGER :: IO_Status=0
```

```
   PRINT*,' Type in the coefficients A, B AND C'
   READ(UNIT=*,FMT=*,IOSTAT=IO_Status)A,B,C
   IF (IO_Status == 0) THEN
     OK=.TRUE.
   ELSE
     OK=.FALSE.
   ENDIF
END SUBROUTINE Interact

SUBROUTINE Solve(E,F,G,Root1,Root2,IFail)
   IMPLICIT NONE
   REAL , INTENT(IN) :: E
   REAL , INTENT(IN) :: F
   REAL , INTENT(IN) :: G
   REAL , INTENT(OUT) :: Root1
   REAL , INTENT(OUT) :: Root2
   INTEGER , INTENT(INOUT) :: IFail
! Local variables
   REAL :: Term
   REAL :: A2
   Term = F*F - 4.*E*G
   A2 = E*2.0
! if term < 0, roots are complex
   IF(Term < 0.0)THEN
     IFail=1
   ELSE
     Term = SQRT(Term)
     Root1 = (-F+Term)/A2
     Root2 = (-F-Term)/A2
   ENDIF
END SUBROUTINE Solve
```

The key code is given below:

```
INTERFACE

   SUBROUTINE Interact(A,B,C,OK)
      IMPLICIT NONE
      REAL , INTENT(OUT) :: A
      REAL , INTENT(OUT) :: B
      REAL , INTENT(OUT) :: C
      LOGICAL , INTENT(OUT) :: OK
   END SUBROUTINE Interact
```

```
   SUBROUTINE Solve(E,F,G,Root1,Root2,IFail)
      IMPLICIT NONE
      REAL , INTENT(IN) :: E
      REAL , INTENT(IN) :: F
      REAL , INTENT(IN) :: G
      REAL , INTENT(OUT) :: Root1
      REAL , INTENT(OUT) :: Root2
      INTEGER , INTENT(INOUT) :: IFail
   END SUBROUTINE Solve

END INTERFACE
```

Interface blocks in the above example provide us with the ability to do type checking between the calling routine and the called routine. One of the most common errors in programming is getting the sequence and type of the parameters wrong between subprograms. There is of course the editing overhead of duplicating the code in this example. We will look at software tools that can generate interface blocks for us in a later chapter.

There are times when the use of interface blocks is mandatory in Fortran and we will cover this as and when required. However, it is good working practice to provide interface blocks when dealing with legacy Fortran 77 style code.

We will look at additional ways of providing explicit interfaces later on.

As Fortran 95 libraries become more widely available interface blocks for library routines will be provided by the supplier on line, and this minimises much of the effort in using them. Nag, for example, already has interface blocks available for its library for many platforms.

22.4 Example 4 — Quadratic example and the CONTAINS statement

This example solves the problem of diagnosing mismatches between the calling and called routine by the CONTAINS statement. The two subroutines Interact and Solve are now part of the main program. This method has drawbacks with larger codes suites as we will end up recompiling all of the code within the main program:

```
PROGRAM ch2204
IMPLICIT NONE
! Simple example of the use of a main program and two
! subroutines. One interacts with the user and the
! second solves a quadratic equation,
```

```
! based on the use input.

REAL :: P, Q, R, Root1, Root2
INTEGER :: IFail=0
LOGICAL :: OK=.TRUE.
  CALL Interact(P,Q,R,OK)
  IF (OK) THEN
    CALL Solve(P,Q,R,Root1,Root2,IFail)
    IF (IFail == 1) THEN
      PRINT *,' Complex roots, calculation abandoned'
    ELSE
      PRINT *,' Roots are  ',Root1,'  ',Root2
    ENDIF
  ELSE
    PRINT*,' Error in data input program ends'
  ENDIF

contains

SUBROUTINE Interact(A,B,C,OK)
  IMPLICIT NONE
  REAL , INTENT(OUT) :: A
  REAL , INTENT(OUT) :: B
  REAL , INTENT(OUT) :: C
  LOGICAL , INTENT(OUT) :: OK
  INTEGER :: IO_Status=0
  PRINT*,' Type in the coefficients A, B AND C'
  READ(UNIT=*,FMT=*,IOSTAT=IO_Status)A,B,C
  IF (IO_Status == 0) THEN
    OK=.TRUE.
  ELSE
    OK=.FALSE.
  ENDIF
END SUBROUTINE Interact

SUBROUTINE Solve(E,F,G,Root1,Root2,IFail)
  IMPLICIT NONE
  REAL , INTENT(IN) :: E
  REAL , INTENT(IN) :: F
  REAL , INTENT(IN) :: G
  REAL , INTENT(OUT) :: Root1
  REAL , INTENT(OUT) :: Root2
```

```
   INTEGER , INTENT(INOUT) :: IFail
! Local variables
   REAL :: Term
   REAL :: A2
   Term = F*F - 4.*E*G
   A2 = E*2.0
! if term < 0, roots are complex
   IF(Term < 0.0)THEN
      IFail=1
   ELSE
      Term = SQRT(Term)
      Root1 = (-F+Term)/A2
      Root2 = (-F-Term)/A2
   ENDIF
END SUBROUTINE Solve

END PROGRAM ch2204
```

Thus in this chapter we have seen three ways of using subroutines:

- Classic Fortran 77 style as in the first example. The major disadvantage is the lack of checking of the parameters between the calling and called routine.
- Interface blocks — the major disadvantage is the code duplication
- Contained subroutines — major disadvantage is that we have to recompile the program and all contained subroutines.

We will look at using modules to address this problem in a later chapter.

22.5 Why bother?

Given the increase in the complexity of the overall program to solve a relatively straightforward problem, one must ask why bother. The answer lies in our ability to manage the solution of larger and larger problems. We need all the help we can get if we are to succeed in our task of developing large-scale reliable programs.

We need to be able to break our problems down into manageable subcomponents and solve each in turn. We are now in a very good position to be able to do this. Given a problem that requires a main program, one or more functions and one or more subroutines we can work on each subcomponent in relative isolation, and know that by using features like interface blocks we will be able to glue all of the components together into a stable structure at the end. We can independently compile the main program and functions and subroutines and use the linker to generate the overall executable, and then test that. Providing we keep our interfaces the

same we can alter the actual implementations of the functions and subroutines and just recompile the changed procedures.

22.6 Summary

We now have the following concepts for the use of subroutines:

- INTERFACE blocks.
- INTENT attribute for parameters.
- Dummy parameters.
- The use of the CALL statement to invoke a subroutine.
- The concepts of variables that are local to the called routines and are unavailable elsewhere in the overall program.
- Communication between program units via the argument list.
- The concept of parameters on the call that enable us to report back on the status of the called routine.

22.7 Problems

1. Type in the program example in this chapter as three files. Compile each individually. When you have successfully compiled each routine (there will be the inevitable typing mistakes) look at the file sizes of the object file. Now use the linker to produce one executable. Look at the file size of the executable. What do you notice?

The development of large programs is eased considerably by the ability to compile small program units and eradicate the compilation errors from one unit at a time.

The linker obviously also has an important role to play in the development process.

2. Write a subroutine to calculate new coordinates (x', y') from (x, y) when the axes are rotated counterclockwise through an angle of a radians using:

$$x' = x\cos a + y\sin a$$

$$y' = -x\sin a + y\cos a$$

Hint:

The subroutine would look something like

SUBROUTINE ChangeCoordinate(X,Y,A,XD,YD)

Write a main program to read in values of *x,y,a*, call the subroutine and print out the new coordinates.

23

Subroutines: 2

"It is one thing to show a man he is in error, and another to put him in possession of the truth."

John Locke

Aims

The aims of this chapter are to extend the ideas in the earlier chapter on subroutines and look in more depth at parameter passing, in particular using a variety of ways of passing arrays.

23 Subroutines: 2

23.1 More on parameter passing

So far we have seen scalar parameters of type real, integer and logical. We will now look at numeric array parameters and character parameters. We need to introduce some technical terminology first. Don't panic if you don't fully understand the terminology the as examples should clarify things.

23.1.1 Explicit-shape array

An explicit-shape array is a named array that is declared with explicit values for the bounds in each dimension of the array.

The following explicit-shape arrays can specify nonconstant bounds:

- An automatic array (the array is a local variable).
- An adjustable array (the array is a dummy argument to a subprogram).

23.1.2 Assumed-shape array

An assumed-shape array is a nonpointer dummy argument array that takes its shape from the associated actual argument array.

23.1.3 Deferred-shape array

A deferred-shape array is an allocatable array or an array pointer. An allocatable array is an array that has the ALLOCATABLE attribute and a specified rank, but its bounds, and hence shape, are determined by allocation or argument association.

23.1.4 Automatic arrays

An automatic array is an explicit-shape array that is a local variable. Automatic arrays are only allowed in function and subroutine subprograms, and are declared in the specification part of the subprogram. At least one bound of an automatic array must be a nonconstant specification expression. The bounds are determined when the subprogram is called.

23.1.5 Assumed-size array — Fortran 77 style

An assumed-size array is a dummy argument array whose size is assumed from that of an associated actual argument. The rank and extents may differ for the actual and dummy arrays; only the size of the actual array is assumed by the dummy array. You would not use this type of parameter in modern Fortran code. We will come back to arrays of this type in the chapter on converting from Fortran 77 to modern Fortran.

23.1.6 Adjustable arrays — Fortran 77 style

An adjustable array is an explicit-shape array that is a dummy argument to a subprogram. At least one bound of an adjustable array must be a nonconstant specification expression. The bounds are determined when the subprogram is called. You would not use this type of parameter in modern Fortran code. We will come back to arrays of this type in the chapter on converting from Fortran 77 to modern Fortran.

23.2 Common code example

We are going to use an example based on a main program and a subroutine that calculates the mean and standard deviation of an array of numbers. The subroutine has the following parameters:

- x - the array containing the real numbers.
- n - the number of elements in the array.
- mean - the mean of the numbers.
- std_dev - the standard deviaition of the numbers.

We will look at some of the ways we can pass the array between the main program and the subroutine in both Fortran 77 and Fortran 90 styles.

23.3 Explicit-shape example

Consider the following program and subroutine.

```
program ch2301
implicit none
integer , parameter        :: n=10
real , dimension(1:n)      :: x
real , dimension(-4:5)     :: y
real , dimension(10)       :: z
real , allocatable , dimension(:) :: t
real :: m,sd
integer :: i

interface
  subroutine stats(x,n,mean,std_dev)
    implicit none
    integer , intent(in)                    :: n
    real    , intent(in) , dimension(1:n)   :: x
    real    , intent(out)                    :: mean
    real    , intent(out)                    :: std_dev
```

```
   end subroutine stats
end interface

   do i=1,n
     x(i)=real(i)
   end do
   call stats(x,n,m,sd)
   print *,' x'
   print *,' mean = ',m
   print *,' Standard deviation = ',sd
   y=x
   call stats(y,n,m,sd)
   print *,' y'
   print *,' mean = ',m
   print *,' Standard deviation = ',sd
   z=x
   call stats(z,10,m,sd)
   print *,' z'
   print *,' mean = ',m
   print *,' Standard deviation = ',sd
   allocate(t(10))
   t=x
   call stats(t,10,m,sd)
   print *,' t'
   print *,' mean = ',m
   print *,' Standard deviation = ',sd
end program ch2301

subroutine stats(x,n,mean,std_dev)
implicit none
integer , intent(in)                        :: n
real    , intent(in) , dimension(1:n) :: x
real    , intent(out)                       :: mean
real    , intent(out)                       :: std_dev
real :: variance
real:: sumxi,sumxi2
integer :: i

   variance=0.0
   sumxi=0.0
   sumxi2=0.0
   do i=1,n
```

```
      sumxi = sumxi+ x(i)
      sumxi2 = sumxi2 + x(i)*x(i)
   end do
   mean=sumxi/n
   variance = (sumxi2 - sumxi*sumxi/n)/(n-1)
   std_dev=sqrt(variance)
end subroutine stats
```

The key line in the subroutine is

```
real     , intent(in) , dimension(1:n) :: x
```

where the dummy array argument x is declared with explicit bounds and known as an explicit-shape dummy array. Even though it is not mandatory it is recommended that interface blocks be used so that the shape and size of actual and dummy arguments can be checked explicitly.

Note also the use of a DO loop to calculate the sum of the elements and the sum of the squares of the elements. This is a Fortran 77 style solution to this problem.

23.4 Assumed-shape example

A fundamental rule in modern Fortran is that the shape of an actual array argument and its associated dummy arguments are the same, i.e., they both must have the same rank and the same extents in each dimension. The best way to apply this rule is to use assumed-shape dummy array arguments as shown in the example below.

In the subroutine we have

```
real , intent(in) , dimension(:) :: x
```

where x is an assumed-shape dummy array argument, and it will assume the shape of the actual argument when the subroutine is called.

In this example in the main program we have declared the actual array argument x to be allocatable to make the program more flexible.

```
program ch2302

implicit none
integer                                :: n
real , allocatable , dimension(:)   :: x
real :: m,sd

interface
   subroutine stats(x,n,mean,std_dev)
```

```
     implicit none
     integer , intent(in)                  :: n
     real    , intent(in) , dimension(:) :: x
     real    , intent(out)                 :: mean
     real    , intent(out)                 :: std_dev
   end subroutine stats
end interface

   print *,' type in n'
   read *,n
   allocate(x(1:n))
   call random_number(x)
   x=x*100
   call stats(x,n,m,sd)
   print *,' numbers were '
   print *,x
   print *,' Mean =                    ',m
   print *,' Standard deviation = ',sd

end program ch2302

subroutine stats(x,n,mean,std_dev)
implicit none
integer , intent(in)                    :: n
real    , intent(in) , dimension(:)    :: x
real    , intent(out)                   :: mean
real    , intent(out)                   :: std_dev
real :: variance
real:: sumxi,sumxi2
integer :: i

   variance=0.0
   sumxi=0.0
   sumxi2=0.0
   do i=1,n
      sumxi = sumxi+ x(i)
      sumxi2 = sumxi2 + x(i)*x(i)
   end do
   mean=sumxi/n
   variance = (sumxi2 - sumxi*sumxi/n)/(n-1)
   std_dev=sqrt(variance)
end subroutine stats
```

23.4.1 Notes

There are several restrictions when using assumed-shape arrays:

- The rank is equal to the number of colons, in this case 1.
- The lower bounds of the assumed-shape array are the specified lower bounds, if present, and 1 otherwise. In the example above it is 1 because we haven't specified a lower bound.
- The upper bounds will be determined on entry to the procedure and will be whatever values are needed to make sure that the extents along each dimension of the dummy argument are the same as the actual argument. In this case the upper bound will be n.
- An assumed-shape array must not be defined with the POINTER or ALLOCATABLE attribute in Fortran 90 or Fortran 95.
- When using an assumed-shape array an interface block is mandatory.

Assumed-shape arraay parameter passing also works with Fortran 77 style statically allocated arrays, i.e.,

```
real , dimension(1:10) :: x
```

which is commonly seen in older code.

23.5 Character arguments and assumed-length dummy arguments

The types of parameters considered so far have been REAL, INTEGER and LOGICAL. CHARACTER variables are slightly different because they have a length associated with them. Consider the following program and subroutine which, given the name of a file, opens it and reads values into two REAL arrays, X and Y:

```
PROGRAM ch2303
IMPLICIT NONE
REAL,DIMENSION(1:100)::A,B
INTEGER :: Nos,I
CHARACTER(LEN=20)::Filename
INTERFACE
   SUBROUTINE Readin(Name,X,Y,N)
      IMPLICIT NONE
      INTEGER , INTENT(IN) :: N
      REAL,DIMENSION(1:N),INTENT(OUT)::X,Y
      CHARACTER (LEN=*),INTENT(IN)::Name
   END SUBROUTINE Readin
```

```
END INTERFACE
   PRINT *,' Type in the name of the data file'
   READ '(A)' , Filename
   PRINT *,' Input the number of items in the file'
   READ * , Nos
   CALL Readin(Filename,A,B,Nos)
   PRINT * , ' Data read in was'
   DO I=1,Nos
      PRINT *,' ',A(I),' ',B(I)
   ENDDO

END PROGRAM ch2303

SUBROUTINE Readin(Name,X,Y,N)
IMPLICIT NONE
INTEGER , INTENT(IN) :: N
REAL,DIMENSION(1:N),INTENT(OUT)::X,Y
CHARACTER (LEN=*),INTENT(IN)::Name
INTEGER::I
   OPEN(UNIT=10,STATUS='OLD',FILE=Name)
   DO I=1,N
      READ(10,*)X(I),Y(I)
   END DO
   CLOSE(UNIT=10)
END SUBROUTINE Readin
```

The main program reads the file name from the user and passes it to the subroutine that reads in the data. The dummy argument Name is of type assumed-length, and picks up the length from the actual argument Filename in the calling routine, which is in this case 20 characters. An interface block **must** be used with assumed-shape dummy arguments.

23.6 Rank 2 and higher arrays as parameters

23.6.1 Explicit-shape dummy arrays

Consider the following example which uses a Fortran 77 style of two-dimensional array parameter passing.

In the main program we have the following declaration of the rank 2 actual array arguments:

```
REAL   , DIMENSION (1:Max,1:Max)::One,Two,Three,One_T
```

and in the subroutine Matrix_bits we declare the rank 2 dummy array arguments as follows:

```
REAL, DIMENSION (1:Max,1:Max), INTENT(IN) :: A,B
REAL, DIMENSION (1:Max,1:Max), INTENT(OUT) :: C,A_T
```

We have split the declaration into two as the arrays have different intents. These dummy array arguments are explicit-shape, i.e., their bounds are declared in the subroutine.

Note that in the main program N may be less than Max and because of the way Fortran stores arrays internally we must pass both variables as arguments to the subroutine Matrix_bits, N being used to control the DO loops and Max needed in the array declarations:

```
PROGRAM ch2304
IMPLICIT NONE
INTEGER, PARAMETER :: Max=10
REAL   , DIMENSION (1:Max,1:Max)::One,Two,Three,One_T
INTEGER :: I,N
INTERFACE
  SUBROUTINE Matrix_bits(A,B,C,A_T,N,Max)
  IMPLICIT NONE
  INTEGER, INTENT(IN):: N, Max
  REAL, DIMENSION (1:Max,1:Max), INTENT(IN) :: A,B
  REAL, DIMENSION (1:Max,1:Max), INTENT(OUT) :: C,A_T
  END SUBROUTINE Matrix_bits
END INTERFACE

    PRINT *,'Input size of matrices'
    READ*,N
    DO WHILE(N > Max)
      PRINT*,'size of matrices must be <= ',Max
      PRINT *,'Input size of matrices'
    READ*,N
    END DO
    DO I=1,N
      PRINT*, 'Input row ', I,' of One'
      READ*,One(I,1:N)
    END DO
    DO I=1,N
      PRINT*, 'Input row ', I,' of Two'
      READ*,Two(I,1:N)
    END DO
```

```
     CALL Matrix_bits(One,Two,Three,One_T,N,Max)
     PRINT*,' Matrix Three:'
     DO I=1,N
        PRINT *,Three(I,1:N)
     END DO
     PRINT *,' Matrix One_T:'
     DO I=1,N
        PRINT *,One_T(I,1:N)
     END DO
END PROGRAM ch2304

SUBROUTINE Matrix_bits(A,B,C,A_T,N,Max)
IMPLICIT NONE
INTEGER, INTENT(IN):: N, Max
REAL, DIMENSION (1:Max,1:Max), INTENT(IN) :: A,B
REAL, DIMENSION (1:Max,1:Max), INTENT(OUT) :: C,A_T

INTEGER::I,J,K
REAL:: Temp
!
! matrix multiplication C=A B
!
    DO I=1,N
        DO J=1,N
            Temp=0.0
            DO K=1,N
                Temp = Temp + A(I,K) * B (K,J)
            END DO
                C(I,J) = Temp
        END DO
    END DO
!
! set A_T to be transpose matrix A
   DO I=1,N
       DO J=1,N
           A_T(I,J) = A(J,I)
       END DO
 END DO
END SUBROUTINE Matrix_bits
```

Note the use of DO loops to carry out the matrix multiplication and transpose. This is a Fortran 77 style solution to the problem.

23.6.2 Assumed-shape dummy array arguments

With the introduction of assumed-shape dummy array arguments the necessity to pass through Max in the last program is removed. This is shown in the example below:

```
PROGRAM ch2305
   IMPLICIT NONE
   REAL , ALLOCATABLE , DIMENSION &
   (:,:)::One,Two,Three,One_T
   INTEGER :: I,N
   INTERFACE
      SUBROUTINE Matrix_bits(A,B,C,A_T,N)
      IMPLICIT NONE
      INTEGER, INTENT(IN):: N
         REAL, DIMENSION (:,:), INTENT(IN) :: A,B
         REAL, DIMENSION (:,:), INTENT(OUT) :: C,A_T
      END SUBROUTINE Matrix_bits
   END INTERFACE
      PRINT *,'Input size of matrices'
      READ*,N
      ALLOCATE(One(1:N,1:N))
      ALLOCATE(Two(1:N,1:N))
      ALLOCATE(Three(1:N,1:N))
      ALLOCATE(One_T(1:N,1:N))
      DO I=1,N
         PRINT*, 'Input row ', I,' of One'
         READ*,One(I,1:N)
      END DO
      DO I=1,N
         PRINT*, 'Input row ', I,' of Two'
         READ*,Two(I,1:N)
      END DO
      CALL Matrix_bits(One,Two,Three,One_T,N)
      PRINT*,' Matrix Three:'
      DO I=1,N
         PRINT *,Three(I,1:N)
      END DO
      PRINT *,' Matrix One_T:'
      DO I=1,N
         PRINT *,One_T(I,1:N)
      END DO
END PROGRAM ch2305
```

```
SUBROUTINE Matrix_bits(A,B,C,A_T,N)
   IMPLICIT NONE
   INTEGER, INTENT(IN):: N
   REAL, DIMENSION (:,:), INTENT(IN) :: A,B
   REAL, DIMENSION (:,:), INTENT(OUT) :: C,A_T
   INTEGER:: I,J, K
   REAL:: Temp
!
! matrix multiplication C=AB
!
    DO I=1,N
        DO J=1,N
            Temp=0.0
            DO K=1,N
                Temp = Temp + A(I,K) * B (K,J)
            END DO
                C(I,J) = Temp
        END DO
    END DO
!
! Calculate A_T transpose of A
!
!
! set A_T to be transpose matrix A
   DO I=1,N
       DO J=1,N
           A_T(I,J) = A(J,I)
       END DO
 END DO
END SUBROUTINE Matrix_bits
```

23.6.3 Notes

The dummy array and actual array arguments look the same but there is a difference:

- The dummy array arguments A, B, C, A_T are all assumed-shape arrays and take the shape of the actual array arguments One, Two, Three and One_T, respectively.
- The actual array arguments One, Two, Three and One_T in the main program are allocatable arrays or deferred-shape arrays. An allocatable array

is an array that has an allocatable attribute. Its bounds and shape are declared when the array is allocated, hence deferred-shape.

23.6.4 Using the intrinsic functions MATMUL and TRANSPOSE

In the previous two examples the matrix multiplication and transpose were hand coded, and are what you would see in Fortran 77 style code. This example uses the built in intrinsics MATMUL and TRANSPOSE and is modern Fortran 90 style:

```
PROGRAM ch2306
  IMPLICIT NONE
  REAL , ALLOCATABLE , DIMENSION &
  (:,:)::One,Two,Three,One_T
  INTEGER :: I,N
  INTERFACE
    SUBROUTINE Matrix_bits(A,B,C,A_T)
      IMPLICIT NONE
      REAL, DIMENSION (:,:), INTENT(IN) :: A,B
      REAL, DIMENSION (:,:), INTENT(OUT) :: C,A_T
    END SUBROUTINE Matrix_bits
  END INTERFACE
    PRINT *,'Input size of matrices'
    READ*,N
    ALLOCATE(One(1:N,1:N))
    ALLOCATE(Two(1:N,1:N))
    ALLOCATE(Three(1:N,1:N))
    ALLOCATE(One_T(1:N,1:N))
    DO I=1,N
      PRINT*, 'Input row ', I,' of One'
      READ*,One(I,1:N)
    END DO
    DO I=1,N
      PRINT*, 'Input row ', I,' of Two'
      READ*,Two(I,1:N)
    END DO
    CALL Matrix_bits(One,Two,Three,One_T)
    PRINT*,' Matrix Three:'
    DO I=1,N
      PRINT *,Three(I,1:N)
    END DO
    PRINT *,' Matrix One_T:'
    DO I=1,N
      PRINT *,One_T(I,1:N)
    END DO
```

```
END PROGRAM ch2306

SUBROUTINE Matrix_bits(A,B,C,A_T)
   IMPLICIT NONE
   REAL, DIMENSION (:,:), INTENT(IN) :: A,B
   REAL, DIMENSION (:,:), INTENT(OUT) :: C,A_T
      C=MATMUL(A,B)
      A_T=TRANSPOSE(A)
END SUBROUTINE Matrix_bits
```

Fortran thus provides a variety of ways of passing array parameters. We have covered both 77 and 90 styles, as you will see both in code that you work with.

23.7 Automatic arrays and median calculation

This example looks at the calculation of the median of a set of numbers and also illustrates the use of an automatic array.

The median is the middle value of a list, i.e., the smallest number such that at least half the numbers in the list are no greater. If the list has an odd number of entries, the median is the middle entry in the list after sorting the list into ascending order. If the list has an even number of entries, the median is equal to the sum of the two middle (after sorting) numbers divided by two. One way to determine the median computationally is to sort the numbers and choose the item in the middle.

Wirth classifies sorting into simple and advanced, and his three simple methods are as follows:

- Insertion sorting — The items are considered one at a time and each new item is inserted into the appropriate position relative to the previously sorted item. If you have ever played bridge then you have probably used this method.
- Selection sorting — First the smallest (or largest) item is chosen and is set aside from the rest. Then the process is repeated for the next smallest item and set aside in the next position. This process is repeated until all items are sorted.
- Exchange sorting — If two items are found to be out of order they are interchanged. This process is repeated until no more exchanges take place.

Knuth also identifies the above three sorting methods. For more information on sorting the Knuth and Wirth books are good starting places. Knuth is a little old (1973) compared to Wirth (1986), but it is still a very good coverage. Knuth uses mix assembler to code the examples whilst the Wirth book uses Modula 2, and is therefore easier to translate into modern Fortran.

In the example below we use a selection sort:

```
program ch2307

implicit none
integer :: n
real , allocatable , dimension(:) :: x
real :: m,sd,median

interface
  subroutine stats(x,n,mean,std_dev,median)
    implicit none
    integer , intent(in)                  :: n
    real    , intent(in) , dimension(:)   :: x
    real    , intent(out)                 :: mean
    real    , intent(out)                 :: std_dev
    real    , intent(out)                 :: median
  end subroutine stats
end interface

  print *,' How many values ?'
  read *,n
  allocate(x(1:n))
  call random_number(x)
  x=x*1000
  call stats(x,n,m,sd,median)
  print *,' mean = ',m
  print *,' Standard deviation = ',sd
  print *,' median is = ',median

end program ch2307

subroutine stats(x,n,mean,std_dev,median)
implicit none
integer , intent(in)                   :: n
real    , intent(in) , dimension(:)    :: x
real    , intent(out)                  :: mean
real    , intent(out)                  :: std_dev
real    , intent(out)                  :: median
real    , dimension(1:n)               :: y
real :: variance
real    :: sumxi, sumxi2
  sumxi=0.0
```

```
   sumxi2=0.0
   variance=0.0
   sumxi=sum(x)
   sumxi2=sum(x*x)
   mean=sumxi/n
   variance=(sumxi2-sumxi*sumxi/n)/(n-1)
    std_dev = sqrt(variance)
   y=x
   call selection
   if (mod(n,2) == 0) then
     median=(y(n/2)+y((n/2)+1))/2
   else
     median=y((n/2)+1)
   endif
contains

   subroutine selection
   implicit none
   integer :: i,j,k
   real :: minimum
     do i=1,n-1
       k=i
       minimum=y(i)
       do j=i+1,n
         if (y(j) < minimum) then
           k=j
           minimum=y(k)
         end if
       end do
       y(k)=y(i)
       y(i)=minimum
     end do
   end subroutine selection

end subroutine stats
```

In the subroutine stats the array y is automatic. It will be allocated automatically when we call the subroutine. We use this array as a work array to hold the sorted data. We then use this sorted array to determine the median.

Note the use of the SUM intrinsic in this example:

```
sumxi=sum(x)
sumxi2=sum(x*x)
```

These statements replace the DO loop from the earlier example. A good optimising compiler would not make two passes over the data with these two statements.

23.7.1 Internal subroutines and scope

The stats subroutine contains the selection subroutine. The stats subroutine has access to the following variables

- x,n,mean,std_dev, median — these are made available as they are passed in as parameters.
- y, variance, sumxi, sumxi2 — are local to the subroutine stats.

The subroutine selection has access to the above as it is contained within subroutine stats. It also has the following local variables that are only available within subroutine selection

- i,j,k, minimum

23.7.2 Timing the selection sort algorithm

The selection sort is a simple algorithm and the following main program illustrates it limitations with increasing n. It uses the same stats subroutine as the previous example:

```
program ch2308

implicit none
integer :: n
real , allocatable , dimension(:) :: x
real :: m,sd,median
integer , dimension(8) :: timing

interface
  subroutine stats(x,n,mean,std_dev,median)
    implicit none
    integer , intent(in)                    :: n
    real    , intent(in) , dimension(:)     :: x
    real    , intent(out)                     :: mean
    real    , intent(out)                     ::
std_dev
    real    , intent(out)                     :: median
  end subroutine stats
end interface
```

```
  n=1000
  do
    print *,' n = ',n
    allocate(x(1:n))
    call random_number(x)
    x=x*1000
    call date_and_time(values=timing)
    print *,' initial '
    print *, timing(6) , timing(7) , timing(8)
    call stats(x,n,m,sd,median)
    print *,' mean = ',m
    print *,' Standard deviation = ',sd
    print *,' median is = ',median
    call date_and_time(values=timing)
    print *,' after'
    print *,timing(6),timing(7),timing(8)
    n=n*10
    deallocate(x)
  end do

end program ch2308
```

23.7.2.1 Timing

Dell Precision Workstation, 2 * 933 MHz, 512 Mb ram:

```
  n =  1000
  initial                                    9 13 906
  mean =     5.0895782E+02
  Standard deviation =     2.8708249E+02
  median is =     5.1872925E+02
  after sort                                 9 13 950
  n =  10000
  initial                                    9 13 951
  mean =     4.9967194E+02
  Standard deviation =     2.8635922E+02
  median is =     5.0259839E+02
  after sort                                 9 14 689
  n =  100000
  initial                                    9 14 697
  mean =     5.0123392E+02
  Standard deviation =     2.8869482E+02
  median is =     4.9957404E+02
```

```
  after sort                                    11 12 292
```

Dell Inspiron, 1 * 3.4 Ghz, 1 Gb ram:

```
  n =  1000
  initial                                       10 57 421
  mean =     5.0781586E+02
  Standard deviation =     2.9026807E+02
  median is =     5.1530060E+02
  after sort                                    10 57 524
  n =  10000
  initial                                       10 57 525
  mean =     4.9770724E+02
  Standard deviation =     2.8532513E+02
  median is =     4.9151331E+02
  after sort                                    10 57 778
  n =  100000
  initial                                       10 57 781
  mean =     4.9930457E+02
  Standard deviation =     2.8866571E+02
  median is =     4.9931268E+02
  after sort                                    11 23 374
```

This algorithm is approximately order n * log(n).

23.8 Alternative median calculation algorithm

This program uses an algorithm developed by Hoare to determine the median. The number of computations required to find the median is approximately 2 * n.

Timings are given at the end:

```
program ch2309

implicit none
integer :: n
real , allocatable , dimension(:) :: x
real :: m,sd,median
integer , dimension(8) :: timing

interface
  subroutine stats(x,n,mean,std_dev,median)
    implicit none
    integer , intent(in)                    :: n
```

```
    real     , intent(in) , dimension(:)    :: x
    real     , intent(out)                  :: mean
    real     , intent(out)                  :: std_dev
    real     , intent(out)                  :: median
  end subroutine stats
end interface

  n=1000
  do
    print *,' n = ',n
    allocate(x(1:n))
    call random_number(x)
    x=x*1000
    call date_and_time(values=timing)
    print *,' initial '
    print *,timing(6),timing(7),timing(8)
    call stats(x,n,m,sd,median)
    print *,' mean = ',m
    print *,' Standard deviation = ',sd
    print *,' median is = ',median
    call date_and_time(values=timing)
    print *,' after sort'
    print *, timing(6),timing(7),timing(8)
    n=n*10
    deallocate(x)
  end do

end program ch2309

subroutine stats(x,n,mean,std_dev,median)
implicit none
integer , intent(in)                    :: n
real     , intent(in) , dimension(:)    :: x
real     , intent(out)                  :: mean
real     , intent(out)                  :: std_dev
real     , intent(out)                  :: median
real     , dimension(1:n)               :: y
real :: variance
real     :: sumxi, sumxi2
integer:: k
  sumxi=0.0
  sumxi2=0.0
```

```
variance=0.0
sumxi=sum(x)
sumxi2=sum(x*x)
mean=sumxi/n
variance=(sumxi2-sumxi*sumxi/n)/(n-1)
std_dev = sqrt(variance)
y=x
if (mod(n,2) == 0) then
  median = ( find(n/2)+find((n/2)+1) )/2
else
  median=find((n/2)+1)
endif

contains

  real function find(k)
  implicit none
  integer , intent(in) :: k
  integer :: l,r,i,j
  real :: t1,t2
    l=1
    r=n
    do while (l<r)
      t1=y(k)
      i=l
      j=r
      do
        do while (y(i)<t1)
          i=i+1
        end do
        do while (t1<y(j))
          j=j-1
        end do
        if (i<=j) then
          t2=y(i)
          y(i)=y(j)
          y(j)=t2
          i=i+1
          j=j-1
        end if
        if (i>j) exit
      end do
```

```
          if (j<k) then
            l=i
          end if
          if (k<i) then
            r=j
          end if
        end do
        find=y(k)
      end function find

end subroutine stats
```

23.8.1 Timing

Dell Precision Workstation, 2 * 933 MHz, 512 Mb ram:

```
 n =  1000
 initial                                  19 37 421
 mean =     4.9430524E+02
 Standard deviation =     2.9318149E+02
 median is =     4.8815854E+02
 after sort                               19 37 426
 n =  10000
 initial                                  19 37 427
 mean =     4.9803854E+02
 Standard deviation =     2.9065613E+02
 median is =     4.9482861E+02
 after sort                               19 37 431
 n =  100000
 initial                                  19 37 439
 mean =     5.0035132E+02
 Standard deviation =     2.8867920E+02
 median is =     5.0099771E+02
 after sort                               19 37 468
 n =  1000000
 initial                                  19 37 542
 mean =     4.9944907E+02
 Standard deviation =     2.8857736E+02
 median is =     4.9952847E+02
 after sort                               19 37 838
 n =  10000000
 initial                                  19 38 626
 mean =     4.9974246E+02
 Standard deviation =     2.8268231E+02
```

```
median is =     4.9996432E+02
after sort                                  19 41 722
```

Dell Inspiron, 1 * 3.4 Ghz, 1 Gb ram:

```
n =  1000
initial                                     21 38 734
mean =     4.9351086E+02
Standard deviation =     2.9076068E+02
median is =     4.8678186E+02
after sort                                  21 38 734
n =  10000
initial                                     21 38 734
mean =     5.0000485E+02
Standard deviation =     2.8909946E+02
median is =     4.9666431E+02
after sort                                  21 38 765
n =  100000
initial                                     21 38 768
mean =     5.0053433E+02
Standard deviation =     2.8863885E+02
median is =     4.9899475E+02
after sort                                  21 38 775
n =  1000000
initial                                     21 38 797
mean =     5.0039590E+02
Standard deviation =     2.8852356E+02
median is =     5.0053967E+02
after sort                                  21 38 855
n =  10000000
initial                                     21 39 67
mean =     4.9973923E+02
Standard deviation =     2.8260712E+02
median is =     4.9987134E+02
after sort                                  21 39 806
n =  100000000
initial                                     21 41 930
mean =     1.7179869E+02
Standard deviation =     3.8263177E+02
median is =     5.0002957E+02
after sort                                  21 59 222
```

The differences between the two algorithms and systems are summarised below:

System	N	Selection	Find
Dual	100,000,000	NA	NA
	10,000,000	NA	3.096
	1,000,000	NA	0.296
	100,000	117.595	0.029
	10,000	0.738	0.004
Single	100,000,000	NA	17.292
	10,000,000	NA	0.739
	1,000,000	NA	0.058
	100,000	25.593	NA
	10,000	0.253	NA

Hoare's Find algorithm is obviously much faster, but far less easy to understand than the simple selection sort.

The limiting factor with this algorithm on these systems is the amount of installed memory. The program crashes on both systems with a failure to allocate the automatic array. This is a drawback of automatic arrays in that there is no mechanism to handle this failure gracefully.You would then need to use allocatable local work arrays. The drawback here is that the programmer is then responsible for the deallocation of these arrays. Memory leaks are then possible.

23.9 Recursive subroutines — Quicksort

In Chapter 14 we saw an example of recursive functions. This example illustrates the use of recursive subroutines. It uses a simple implementation of Hoare's Quicksort. References are given in the bibliography. The overall problem is broken down into:

- A main program that prompts the user for the name of the data file and n. The allocation of the array is carried out in the main program.
- A subroutine to read the data.
- A subroutine to sort the data. This subroutine contains the recursive subroutine Quicksort.
- A subroutine to write the sorted data to a file.

Below is the complete program:

```
PROGRAM ch2310
IMPLICIT NONE
INTEGER                                        :: How_Many
CHARACTER    (LEN=20)                        :: File_Name
REAL , ALLOCATABLE , DIMENSION(:)   :: Raw_Data
integer , dimension(8) :: timing

INTERFACE
  SUBROUTINE Read_Data(File_Name,Raw_Data,How_Many)
    IMPLICIT NONE
    CHARACTER (LEN=*) , INTENT(IN) :: File_Name
    INTEGER , INTENT(IN) :: How_Many
    REAL , INTENT(OUT) , &
    DIMENSION(:) :: Raw_Data
  END SUBROUTINE Read_Data
END INTERFACE

INTERFACE
  SUBROUTINE Sort_Data(Raw_Data,How_Many)
    IMPLICIT NONE
    INTEGER , INTENT(IN) :: How_Many
    REAL , INTENT(INOUT) , &
    DIMENSION(:) :: Raw_Data
  END SUBROUTINE Sort_Data
END INTERFACE

INTERFACE
  SUBROUTINE Print_Data(Raw_Data,How_Many)
    IMPLICIT NONE
    INTEGER , INTENT(IN) :: How_Many
    REAL , INTENT(IN) , &
    DIMENSION(:) :: Raw_Data
  END SUBROUTINE Print_Data
END INTERFACE

  PRINT * , ' How many data items are there?'
  READ  * , How_Many
  PRINT * , ' What is the file name?'
  READ '(A)',File_Name
  call date_and_time(values=timing)
  print *,' initial'
  print *,timing(6),timing(7),timing(8)
```

```
   ALLOCATE(Raw_Data(How_Many))
   call date_and_time(values=timing)
   print *,' allocate'
   print *,timing(6),timing(7),timing(8)
   CALL Read_Data(File_Name,Raw_Data,How_Many)
   call date_and_time(values=timing)
   print *,' read'
   print *,timing(6),timing(7),timing(8)
   CALL Sort_Data(Raw_Data,How_Many)
   call date_and_time(values=timing)
   print *,' sort'
   print *,timing(6),timing(7),timing(8)
   CALL Print_Data(Raw_Data,How_Many)
   call date_and_time(values=timing)
   print *,' print'
   print *,timing(6),timing(7),timing(8)
   PRINT * , ' '
   PRINT *, ' Data written to file SORTED.DAT'

END PROGRAM ch2310

SUBROUTINE Read_Data(File_Name,Raw_Data,How_Many)
IMPLICIT NONE
CHARACTER (LEN=*) , INTENT(IN) :: File_Name
INTEGER , INTENT(IN) :: How_Many
REAL , INTENT(OUT) , DIMENSION(:) :: Raw_Data
! Local variables
INTEGER :: I

   OPEN(FILE=File_Name,UNIT=1)
   DO I=1,How_Many
     READ (UNIT=1,FMT=*) Raw_Data(I)
   ENDDO

END SUBROUTINE Read_Data

SUBROUTINE Sort_Data(Raw_Data,How_Many)
IMPLICIT NONE
INTEGER , INTENT(IN) :: How_Many
REAL , INTENT(INOUT) , DIMENSION(:) :: Raw_Data

   CALL QuickSort(1,How_Many)
```

```
CONTAINS

   RECURSIVE SUBROUTINE QuickSort(L,R)
   IMPLICIT NONE
   INTEGER , INTENT(IN) :: L,R
   ! Local variables
   INTEGER :: I,J
   REAL :: V,T

   i=l
   j=r
   v=raw_data( int((l+r)/2) )
   do
      do while (raw_data(i) < v )
           i=i+1
      enddo
      do while (v < raw_data(j) )
           j=j-1
      enddo
      if (i<=j) then
         t=raw_data(i)
         raw_data(i)=raw_data(j)
         raw_data(j)=t
         i=i+1
         j=j-1
      endif
      if (i>j) exit
   enddo

   if (l<j) then
      call quicksort(l,j)
   endif

   if (i<r) then
      call quicksort(i,r)
   endif

   END SUBROUTINE QuickSort

END SUBROUTINE Sort_Data
```

```
SUBROUTINE Print_Data(Raw_Data,How_Many)
IMPLICIT NONE
INTEGER , INTENT(IN) :: How_Many
REAL , INTENT(IN) , DIMENSION(:) :: Raw_Data
! Local variables
INTEGER :: I
   OPEN(FILE='SORTED.DAT',UNIT=2)
   DO I=1,How_Many
      WRITE(UNIT=2,FMT=*) Raw_Data(I)
   ENDDO
   CLOSE(2)
END SUBROUTINE Print_Data
```

23.9.1 Note — Interface blocks

We introduced interface blocks in Chapter 22, and in that chapter the parameters were scalars; in this example we have a mix of arrays and scalars. The above program is in Fortran 77 style with a main program and several distinct subroutines. The use of interface blocks is recommended when using this style of programming as it will minimise cross program unit (program, function, subroutine) errors.

Interface blocks are **mandatory** under the following situations:

- The procedure has optional arguments.
- When a function returns an array.
- When a function returns a pointer.
- For character functions a result that is dynamic.
- When the procedure has assumed-shape dummy arguments.
- When the procedure has dummy arguments with the pointer attribute.
- When the procedure has dummy arguments with the target attribute.
- When the procedure has keyword arguments and/or optional arguments.
- When the procedure is generic. You have already seen that some of the intrinsic procedures have this status, e.g., SINE will return a result when the argument is of a variety of types. This means that we can construct procedures that will accept arguments of a variety of types and all we need to do is provide a procedure that manipulates data of that type. We will look at the construction of a procedure that is generic in a later chapter.
- When the procedure provides a user defined operator.

- When the procedure provides user defined assignment.

23.9.2 Note — Recursive subroutine

The actual sorting is done in the recursive subroutine `QuickSort`. The actual algorithm is taken from the Wirth book. See the bibliography for a reference.

Recursion provides us with a very clean and expressive way of solving many problems. There will be instances where it is worthwhile removing the overhead of recursion, but the first priority is the production of a program that is correct. It is pointless having a very efficient but incorrect solution.

We will look again at recursion and efficiency in a later chapter and see under what criteria we can replace recursion with iteration.

23.9.3 Note — Flexible design

The QuickSort recursive routine can be replaced with another sorting algorithm and we can maintain the interface to Sort_Data. We can thus decouple the implementation of the actual sorting routine from the defined interface. We would only need to recompile the Sort_Data routine and we could relink using the already compiled main, read data and print data routines.

23.9.4 Note — Timing information

We call the date_and_time intrinsic subroutine to get timing information. A summary table from runnning the above program on a 3.4 Ghz system with 1 Gb memory with four different compilers is given below:

```
                    n=10,000,000
Compiler
              read      sort      print
1             7.328     2.812     61.391
2             7.563     2.922     58.843
3             5.765     3.281     17.751
4             7.015     3.438     22.344
```

As can be seen it is the I/O that dominates the overall running time of the program. In the 10 years since first running this program we have seen the data set size increase from tens of thousands to tens and hundreds of millions.

23.10 Summary

We now have a lot of the tools to start tackling problems in a structured and modular way, breaking problems down into manageable chunks and designing subprograms for each of the tasks.

23.11 Problems

1. Below is the random number program that was used to generate the data sets for the Quicksort example:

```
program ch2311
implicit none
integer :: n
integer :: i
real , allocatable , dimension(:) :: x
  print *,' how many values ?'
  read *,n
  allocate(x(1:n))
  call random_number(x)
  x=x*1000
  open(unit=10,file='random.txt')
  do i=1,n
    write(10, 100)x(i)
    100 format(f8.3)
  end do
end program ch2311
```

Run the Quick_Sort program in this chapter with the data file as input. Obtain timing details.

What percentage of the time does the program spend in each subroutine? Is it worth trying to make the sort much more efficient given these timings?

2. Find out if there is a subroutine library like the NAG library available. If there is replace the Quick_Sort recursive subroutine with a suitable routine from that library. What times do you obtain?

3. Try using the operating system SORT command to sort the file. What timing figures do you get now?

Was it worth writing a program?

4. Consider the following program:

```
program ch2312
!
! Program to test array subscript checking
! when the array is passed as an argument.
!
implicit none
integer , parameter :: array_size=10
```

```
integer :: i
integer , dimension(array_size) :: a
  do i=1,array_size
    a(i)=i
  end do
  call sub01(a,array_size)
end program ch2312

subroutine sub01(a,array_size)
implicit none
integer , intent(in) :: array_size
integer , intent(in) , dimension(array_size) :: a
integer :: i
integer :: atotal=0
integer :: rtotal=0
  do i=1,array_size
    rtotal=rtotal+a(i)
  end do
  do i=1,array_size+1
    atotal=atotal+a(i)
  end do
  print *,' Apparent total is ' , atotal
  print *,'      real total is ' , rtotal
end subroutine sub01
```

The key thing to note is that we haven't used interface blocks and we have an error in the subroutine where we go outside the array. Run this program. What answer do you get for the apparent total?

Are there any compiler flags or switches which will enable you to trap this error?

23.12 Bibliography

Hoare C.A.R., *Algorithm 63, Partition; Algorithm 64, Quicksort, p.321; Algorithm 65: FIND*, Comm. of the ACM, 4 p.321–322, 1961.

Hoare C.A.R., *Proof of a Program: FIND*, Comm A.C.M., 13, No 1 (1970) 39–45

Hoare C.A.R., *Proof of a Recursive Program: Quicksort*, Comp. J., 14, No 4 (1971) 391–95.

Knuth D.E., *The Art of Computer Programming*, Volume 3 — *Sorting and Searching*, Addison-Wesley, 1973.

Wirth N., *Algorithms and Data Structures*, Prentice-Hall, 1986.

23.13 Commercial numerical and statistical subroutine libraries

There are two major suppliers of commercial libraries:

- NAG: Numerical Algorithms Group

and

- Visual Numerics

They can be found at:

- http://www.nag.co.uk/

and

- http://www.vni.com/index.html

respectively. Their libraries are written by numerical analysts, and are fully tested and well documented. They are under constant development and available for a wide range of hardware platforms and compilers. Parallel versions are also available.

24

An Introduction to Modules

"Common sense is the best distributed commodity in the world, for every man is convinced that he is well supplied with it."

Descartes

Aims

The aims of this chapter are to look at the facilities found in Fortran provided by modules, in particular:

- The use of a module to aid in the consistent definition of precision throughout a program and subprograms.
- The use of modules for global data.
- The use of modules for derived data types.
- Two examples showing the use of modules with contained proecures and their use to package procedures.
- A complete numerical example solving systems of linear equations using Gaussian elimination.

24 An Introduction to Modules

As summarised in the Chapter 23 we now have the tools to solve many problems using just a main program and one or more external and internal subprograms. Both external and internal subprograms communicate through their argument lists, whilst internal subprograms have access to data in their host program units.

We now introduce another type of program unit, the module, which is probably one of the most important features of Fortran 90. The purpose of modules is quite different from that of subprograms. In their simplest form they exist so that anything required by more than one program unit may be packaged in a module and made available where needed.

The form of a module is

```
MODULE module_name
...
END MODULE module_name
```

and the information contained within it is made available in the program units that need to access it by

```
USE module_name
```

The USE statement must be the first statement after the PROGRAM or SUBROUTINE or FUNCTION statement.

In this chapter we will look at:

- Modules for global data.
- Modules for derived types.
- Modules for explicit interfaces.
- Modules containing procedures.

Modules are another program unit and exist so that anything required by more than one program unit may be packaged in a module and made available where needed.

24.1 Modules for global data

So far the only way that a program unit can communicate with a procedure is through the argument list. Sometimes this is very cumbersome, especially if a number of procedures want access to the same data, and it means long argument lists. The problem can be solved using modules; e.g., by defining the precision to which you wish to work and any constants defined to that precision which may be needed by a number of procedures.

24.2 Modules for precision specification and constant definition

In the following example we use a module to define a parameter Long to specify the precision to which we wish to work, and another for a range of mathematical constants including a value for the parameter π. Note that the parameter π is defined to this working precision. We then import the module defining these parameters into the program units that need them:

```
module precision_definition
   implicit none
   integer , parameter ::
long=selected_real_kind(15,307)
end module precision_definition

module maths_constants
   use precision_definition
   implicit none
   real (long) , parameter :: c = 299792458.0_long
   ! units m s-1
   real (long) , parameter :: &
      e = 2.71828182845904523_long
   real (long) , parameter :: g = 9.812420_long
   ! 9.780 356 m s-2 at sea level on the equator
   ! 9.812 420 m s-2 at sea level in London
   ! 9.832 079 m s-2 at sea level at the poles
   real (long) , parameter :: &
      pi = 3.14159265358979323_long
end module maths_constants

PROGRAM ch2401
   USE Precision_definition
   IMPLICIT NONE
   INTERFACE
      SUBROUTINE Sub1(Radius,Area,Circum)
      USE Precision_definition
      IMPLICIT NONE
      REAL(Long),INTENT(IN)::Radius
      REAL(Long),INTENT(OUT)::Area,Circum
      END SUBROUTINE Sub1
   END INTERFACE
   REAL(Long)::R,A,C
   INTEGER ::I
   DO I=1,10
```

```
     PRINT*,'Radius?'
     READ*,R
     CALL Sub1(R,A,C)
     PRINT *,' For radius    = ',R
     PRINT *,' Area          = ',A
     PRINT *,' Circumference = ',C
   END DO
END PROGRAM ch2401

SUBROUTINE Sub1(Radius,Area,Circum)
   USE Precision_definition
   use maths_constants
   IMPLICIT NONE
   REAL(Long),INTENT(IN)::Radius
   REAL(Long),INTENT(OUT)::Area,Circum
   Area=Pi*Radius*Radius
   Circum=2.0_Long*Pi*Radius
END SUBROUTINE Sub1
```

24.2.1 Note

In this example we wish to work with the precision specified by the kind type parameter Long in the module Precision_definition. In order to do this we use the statement

```
USE precision_definition
```

inside the program unit before any declarations. The kind type parameter Long is then used with all the REAL type declaration e.g.,

```
REAL (Long):: R ,A,C
```

To make sure that all floating point calculations are performed to the working precision specified by Long any constants such as 2.0 in subroutine Sub1 are specified as const_Long e.g.,

```
2.0_Long
```

Note also that we define things once and use them on two occasions, i.e., we define the precision once and use this definition in both the main program and the subroutine.

24.3 Modules for sharing arrays of data

The following example uses one module containing a number of constants and a second module containing an array definition:

```
module data
  implicit none
  integer , parameter    :: n=12
  real , dimension(1:n) :: rainfall
  real , dimension(1:n) :: sorted
end module data

program ch2402
use data
implicit none

  call readdata
  call sortdata
  call printdata

end program ch2402

subroutine readdata
use data
implicit none
integer :: i
character (len=40) :: filename
  print *,' What is the filename ?'
  read *,filename
  open(unit=100,file=filename)
  do i=1,n
    read (100,*) rainfall(i)
  end do
end subroutine readdata

subroutine sortdata
use data
  sorted=rainfall
  call selection

  contains

    subroutine selection
```

```
      implicit none
      integer :: i,j,k
      real :: minimum
        do i=1,n-1
          k=i
          minimum=sorted(i)
          do j=i+1,n
            if (sorted(j) < minimum) then
              k=j
              minimum=sorted(k)
            end if
          end do
          sorted(k)=sorted(i)
          sorted(i)=minimum
        end do
      end subroutine selection

end subroutine sortdata

subroutine printdata
use data
implicit none
integer :: i
  print *,' original data is '
  do i=1,n
    print 100,rainfall(i)
    100 format(1x,f7.1)
  end do
  print *,' Sorted data is '
  do i=1,n
    print 100,sorted(i)
  end do
end subroutine printdata
```

Note that in this example the calls to the subroutines have no parameters. They work with the data contained in the module.

24.4 Modules for derived data types

When using derived data types and passing them as arguments to subroutines, both the actual arguments and dummy arguments must be of the same type, i.e., they must be declared with reference to the same type definition. The only way this can

be achieved is by using modules. The user defined type is declared in a module and each program unit that requires that type **uses** the module.

24.4.1 Person data type

In this example we have a user defined type Person which we wish to use in the main program and pass arguments of this type to the subroutines Read_data and Stats. In order to have the type Person available to two subroutines and the main program we have defined Person in a module Personal_details and then made the module available to each program unit with the statement

```
USE Personal_details
```

We also have the use of an interface block to provide the ability to develop the overall solution in stages:

```
MODULE Personal_details
   IMPLICIT NONE
   TYPE Person
      REAL:: Weight
      INTEGER :: Age
      CHARACTER :: Sex
   END TYPE Person
END MODULE Personal_details

PROGRAM ch2403
   USE Personal_details
   IMPLICIT NONE
   INTEGER ,PARAMETER:: Max_no=100
   TYPE (Person), DIMENSION(1:Max_no) :: Patient
   INTEGER :: No_of_patients
   REAL :: Male_average, Female_average
INTERFACE

   SUBROUTINE Read_data(Data,Max_no,No)
      USE Personal_details
      IMPLICIT NONE
      TYPE (Person), DIMENSION (:), INTENT(OUT):: Data
      INTEGER, INTENT(OUT):: No
      INTEGER, INTENT(IN):: Max_no
   END SUBROUTINE Read_Data

   SUBROUTINE Stats(Data,No,M_a,F_a)
      USE Personal_details
```

```
      IMPLICIT NONE
      TYPE(Person), DIMENSION (:) :: Data
      REAL:: M_a,F_a
      INTEGER :: No
   END SUBROUTINE Stats

END INTERFACE
!
   CALL Read_data(Patient,Max_no,No_of_patients)
   CALL Stats( Patient , No_of_patients , &
               Male_average , Female_average)
   PRINT*, 'Average male weight is ',Male_average
   PRINT*, 'Average female weight is ',Female_average
END PROGRAM ch2403

SUBROUTINE Read_Data(Data,Max_no,No)
   USE Personal_details
   IMPLICIT NONE
   TYPE (PERSON), DIMENSION (:), INTENT(OUT)::Data
   INTEGER, INTENT(OUT):: No
   INTEGER, INTENT(IN):: Max_no
   INTEGER :: I
   DO
      PRINT *,'Input number of patients'
      READ *,No
      IF ( No > 0 .AND. No <= Max_no) EXIT
   END DO
   DO I=1,No
      PRINT *,'For person ',I
      PRINT *,'Weight ?'
      READ*,Data(I)%Weight
      PRINT*,'Age ?'
      READ*,Data(I)%Age
      PRINT*,'Sex ?'
      READ*,Data(I)%Sex
   END DO
END SUBROUTINE Read_Data

SUBROUTINE Stats(Data,No,M_a,F_a)
   USE Personal_details
   IMPLICIT NONE
   TYPE(Person), DIMENSION(:)::Data
```

```
   REAL :: M_a,F_a
   INTEGER:: No
   INTEGER :: I,No_f,No_m
   M_a=0.0; F_a=0.0;No_f=0; No_m =0
   DO I=1,No
      IF ( Data(I)%Sex == 'M' &
      .OR. Data(I)%Sex == 'm') THEN
         M_a=M_a+Data(I)%Weight
         No_m=No_m+1
      ELSEIF(Data(I)%Sex == 'F' &
         .OR. Data(I)%Sex == 'f') THEN
         F_a=F_a +Data(I)%Weight
         No_f=No_f+1
      ENDIF
   END DO
   IF (No_m > 0 ) THEN
      M_a = M_a/No_m
   ENDIF
   IF (No_f > 0 ) THEN
      F_a = F_a/No_f
   ENDIF
END SUBROUTINE Stats
```

24.5 Modules containing procedures — Quicksort example

In this example we rewrite the Quicksort example to use modules. Each subroutine is put into a module on its own. The program is given below:

```
module read_data

contains

   SUBROUTINE Read(File_Name,Raw_Data,How_Many)
   IMPLICIT NONE
   CHARACTER (LEN=*) , INTENT(IN) :: File_Name
   INTEGER , INTENT(IN) :: How_Many
   REAL , INTENT(OUT) , DIMENSION(:) :: Raw_Data

   INTEGER :: I

     OPEN(FILE=File_Name,UNIT=1)
     DO I=1,How_Many
        READ (UNIT=1,FMT=*) Raw_Data(I)
```

```
     ENDDO
   END SUBROUTINE Read

end module read_data

module sort_data

contains

   SUBROUTINE Sort(Raw_Data,How_Many)
   IMPLICIT NONE
   INTEGER , INTENT(IN) :: How_Many
   REAL , INTENT(INOUT) , DIMENSION(:) :: Raw_data

     CALL QuickSort(1,How_Many)

   CONTAINS

     RECURSIVE SUBROUTINE QuickSort(L,R)
     IMPLICIT NONE
     INTEGER , INTENT(IN) :: L,R
     INTEGER :: I,J
     REAL :: V,T

     i=l
     j=r
     v=raw_data( int((l+r)/2) )
     do
       do while (raw_data(i) < v )
            i=i+1
       enddo
       do while (v < raw_data(j) )
            j=j-1
       enddo
       if (i<=j) then
         t=raw_data(i)
         raw_data(i)=raw_data(j)
         raw_data(j)=t
         i=i+1
         j=j-1
       endif
       if (i>j) exit
```

```
      enddo

      if (l<j) then
        call quicksort(l,j)
      endif

      if (i<r) then
        call quicksort(i,r)
      endif

      END SUBROUTINE QuickSort

   END SUBROUTINE Sort

end module sort_data

module print_data

contains

   SUBROUTINE Print(Raw_Data,How_Many)
   IMPLICIT NONE
   INTEGER , INTENT(IN) :: How_Many
   REAL , INTENT(IN) , DIMENSION(:) :: Raw_data
   INTEGER :: I
      OPEN(FILE='SORTED.DAT',UNIT=2)
      DO I=1,How_Many
        WRITE(UNIT=2,FMT=*) Raw_data(I)
      ENDDO
      CLOSE(2)
   END SUBROUTINE Print

end module print_data

PROGRAM ch2404
use read_data
use sort_data
use print_data
IMPLICIT NONE
INTEGER                                    :: How_Many
CHARACTER    (LEN=20)                     :: File_Name
REAL , ALLOCATABLE , DIMENSION(:)   :: Raw_data
```

```
integer , dimension(8)                :: dt

   PRINT * , ' How many data items are there?'
   READ  * , How_Many
   PRINT * , ' What is the file name?'
   READ '(A)',File_Name

   call date_and_time(values=dt)
   PRINT 100 , dt(6),dt(7),dt(8)
   100 FORMAT(' Initial cpu time     = ',3(2x,i10))

   ALLOCATE(Raw_data(How_Many))

   call date_and_time(values=dt)
   PRINT 110 , dt(6),dt(7),dt(8)
   110 FORMAT(' Allocate cpu time    = ',3(2x,i10))

   CALL Read(File_Name,Raw_Data,How_Many)

   call date_and_time(values=dt)
   PRINT 120 , dt(6),dt(7),dt(8)
   120 FORMAT(' Read data cpu time   = ',3(2x,i10))

   CALL Sort(Raw_Data,How_Many)

   call date_and_time(values=dt)
   PRINT 130 , dt(6),dt(7),dt(8)
   130 FORMAT(' Quick sort cpu time = ',3(2x,i10))

   CALL Print(Raw_Data,How_Many)

   call date_and_time(values=dt)
   PRINT 140 , dt(6),dt(7),dt(8)
   140 FORMAT(' Write data cpu time = ',3(2x,i10))

   PRINT * , ' '
   PRINT *, ' Data written to file SORTED.DAT'

END PROGRAM ch2404
```

The keys in this example is that each subroutine is in a module as a contained procedure and we just have three use statements in the main program to make the subroutines available.

Note that we do not now have any interface blocks in this program. The cross unit checking that interface blocks make available is provided automatically when using modules.

24.6 Modules containing procedures — Statistics example

This is a reworking of the statistics subroutine introduced earlier. We now break the subroutine down into three separate functions:

- mean
- std_dev
- median

that are contained within a module. The median function also has its own internal procedure, find.

```
module statistics

contains

  real function mean(x,n)
  implicit none
  integer , intent(in)                    :: n
  real    , intent(in) , dimension(:)     :: x
  integer :: i
  real    :: total
    total=0
    do i=1,n
      total=total+x(i)
    end do
    mean=total/n
  end function mean

  real function std_dev(x,n,mean)
  integer , intent(in)                    :: n
  real    , intent(in) , dimension(:)     :: x
  real    , intent(in)                    :: mean
  real                                    :: variance
    variance=0
    do i=1,n
```

```
      variance=variance + (x(i)-mean)**2
    end do
    variance=variance/(n-1)
    std_dev=sqrt(variance)
  end function std_dev

  real function median(x,n)
  integer , intent(in)                    :: n
  real     , intent(in) , dimension(:)    :: x
  real     , dimension(1:n)               :: y
    y=x
    if (mod(n,2) == 0) then
      median = ( find(n/2)+find((n/2)+1) )/2
    else
      median=find((n/2)+1)
    endif

  contains

    real function find(k)
    implicit none
    integer , intent(in) :: k
    integer :: l,r,i,j
    real :: t1,t2
      l=1
      r=n
      do while (l<r)
        t1=y(k)
        i=l
        j=r
        do
          do while (y(i)<t1)
            i=i+1
          end do
          do while (t1<y(j))
            j=j-1
          end do
          if (i<=j) then
            t2=y(i)
            y(i)=y(j)
            y(j)=t2
            i=i+1
```

```
              j=j-1
            end if
            if (i>j) exit
          end do
          if (j<k) then
            l=i
          end if
          if (k<i) then
            r=j
          end if
        end do
        find=y(k)
      end function find

   end function median

end module statistics

program ch2405

use statistics

implicit none
integer :: n
real , allocatable , dimension(:) :: x
real :: m,sd,med
integer , dimension(8) :: v

   print *,' How many values ?'
   read *,n
   call date_and_time(values=v)
   print *,' initial                ',v(6),v(7),v(8)
   allocate(x(1:n))
   call date_and_time(values=v)
   print *,' allocate               ',v(6),v(7),v(8)
   call random_number(x)
   call date_and_time(values=v)
   print *,' random                 ',v(6),v(7),v(8)
   x=x*1000
   call date_and_time(values=v)
   print *,' output                 ',v(6),v(7),v(8)
   m=mean(x,n)
```

```
   call date_and_time(values=v)
   print *,' mean                    ',v(6),v(7),v(8)
   print *,' mean                  = ',m
   sd=std_dev(x,n,m)
   call date_and_time(values=v)
   print *,' standard deviation    ',v(6),v(7),v(8)
   print *,' Standard deviation = ',sd
   med = median(x,n)
   call date_and_time(values=v)
   print *,' median                  ',v(6),v(7),v(8)
   print *,' median is             = ',med
end program ch2405
```

Note again that we do not need to have explicit interface blocks as the packaging of the procedures within a module provides the interface checking automatically.

The program also has timing code added to allow profiling of the various parts of the program.

24.7 The solution of linear equations using Gaussian elimination

At this stage we have introduced many of the concepts needed to write numerical code, and have included a popular algorithm, Gaussian elimination, together with a main program which uses it and a module to bring together many of the features covered so far.

Finding the solution of a system of linear equations is very common in scientific and engineering problems, either as a direct physical problem or indirectly, for example, as the result of using finite difference methods to solve a partial differential equation. We will restrict ourselves to the case where the number of equations and the number of unknowns are the same. The problem can be defined as:

$$\begin{aligned} &a_{11}x_1 + a_{12}x_2 + \ldots + a_{1n}x_n = b_1 \\ &a_{12}x_2 + a_{22}x_2 + \ldots + a_{2n}x_n = b_2 \\ &\ldots \quad \ldots \quad \ldots \quad \ldots \quad = \ldots \\ &a_{n1}x_1 + a_{n2}x_2 + \ldots + a_{nn}x_n = b_n \end{aligned} \tag{1}$$

or

$$\begin{pmatrix} a_{11} & a_{12} & \ldots & a_{1n} \\ a_{21} & a_{22} & \ldots & a_{2n} \\ \ldots & \ldots & \ldots & \ldots \\ a_{n1} & a_{n2} & \ldots & a_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \ldots \\ x_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \ldots \\ b_n \end{pmatrix}$$

which can be written as:

$$A\ x = b \tag{2}$$

where A is the $n\ x\ n$ coefficient matrix, b is the right-hand-side vector and x is the vector of unknowns. We will also restrict ourselves to the case where A is a general real matrix.

Note that there is a unique solution to (2) if the inverse, A^{-1}, of the coefficient matrix A, exists. However, the system should never be solved by finding A^{-1} and then solving $A^{-1}\ b = x$ because of the problems of rounding error and the computational costs.

A well-known method for solving (2) is Gaussian elimination, where multiples of equations are subtracted from others so that the coefficients below the diagonal become zero, producing a system of the form:

$$\begin{pmatrix} a_{11}^* & a_{12}^* & \dots & a_{1n}^* \\ 0 & a_{22}^* & \dots & a_{2n}^* \\ \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & a_{nn}^* \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \dots \\ x_n \end{pmatrix} = \begin{pmatrix} b_1^* \\ b_2^* \\ \dots \\ b_n^* \end{pmatrix}$$

where A has been transformed into an upper triangular matrix. By a process of *backward substitution* the values of x *drop* out.

The subroutine Gaussian_Elimination implements the Gaussian elimination algorithm with *partial pivoting,* which ensure that the multipliers are less than 1 in magnitude, by interchanging rows if necessary. This is to try and prevent the buildup of errors.

This implementation is based on two LINPACK routines SGEFA and SGESL and a Fortran 77 subroutine written by Tim Hopkins and Chris Phillips and found in their book *Numerical Methods in Practice.*

The matrix A and vector B are passed to the subroutine Gaussian_Elimination and on exit both A and B are overwritten. Mathematically Gaussian elimination is described as working on rows, and using partial pivoting row interchanges may be necessary. Due to Fortran's row element ordering, to implement this algorithm efficiently it works on columns rather than rows by interchanging elements within a column if necessary.

```
MODULE Precisions
INTEGER,PARAMETER:: Long=SELECTED_REAL_KIND(15,307)
END MODULE Precisions

PROGRAM Solve
```

```
   USE Precisions
   IMPLICIT NONE
   INTEGER :: I,N
   REAL (Long), ALLOCATABLE:: A(:,:),B(:),X(:)
   LOGICAL:: Singular

INTERFACE

   SUBROUTINE Gaussian_Elimination(A,N,B,X,Singular)
      USE Precisions
      IMPLICIT NONE
      INTEGER, INTENT(IN)::N
      REAL (Long), INTENT (INOUT) :: A(:,:),B(:)
      REAL (Long), INTENT(OUT)::X(:)
      LOGICAL, INTENT(OUT) :: Singular
   END SUBROUTINE Gaussian_Elimination

END INTERFACE

   PRINT *,'Number of equations?'
   READ *,N
   ALLOCATE(A(1:N,1:N),B(1:N),X(1:N))
   DO I=1,N
      PRINT *,'Input elements of row ',I,' of A'
      READ*,A(I,1:N)
      PRINT*,'Input element ',I,' of B'
      READ *,B(I)
   END DO
   CALL Gaussian_Elimination(A,N,B,X,Singular)
   IF(Singular) THEN
      PRINT*, 'Matrix is singular'
   ELSE
      PRINT*, 'Solution X:'
      PRINT*,X(1:N)
   ENDIF
END PROGRAM Solve

SUBROUTINE Gaussian_Elimination(A,N,B,X,Singular)
! Routine to solve a system Ax=b
! using Gaussian Elimination
! with partial pivoting
```

```
! The code is based on the Linpack routines
! SGEFA and SGESL
! and operates on columns rather than rows!
   USE Precisions
   IMPLICIT NONE
! Matrix A and vector B are over-written
! Arguments
   INTEGER, INTENT(IN):: N
   REAL (Long),INTENT(INOUT):: A(:,:),B(:)
   REAL (Long),INTENT(OUT)::X(:)
   LOGICAL,INTENT(OUT)::Singular
! Local variables
   INTEGER::I,J,K,Pivot_row
   REAL (Long):: Pivot,Multiplier,Sum,Element
   REAL (Long),PARAMETER::Eps=1.E-13_Long
!
! Work through the matrix column by column
!
   DO K=1,N-1
!
!  Find largest element in column K for pivot
!
   Pivot_row = MAXVAL( MAXLOC( ABS( A(K:N,K) ) ) ) &
      + K - 1
!
! Test to see if A is singular
! if so return to main program
!
      IF(ABS(A(Pivot_row,K)) <= Eps) THEN
         Singular=.TRUE.
         RETURN
      ELSE
         Singular = .FALSE.
      ENDIF
!
! Exchange elements in column K if largest is
! not on the diagonal
!
      IF(Pivot_row /= K) THEN
         Element=A(Pivot_row,K)
         A(Pivot_Row,K)=A(K,K)
         A(K,K)=Element
```

```
         Element=B(Pivot_row)
         B(Pivot_row)=B(K)
         B(K)=Element
      ENDIF
!
! Compute multipliers
! elements of column K below diagonal
! are set to these multipliers for use
! in elimination later on
!
      A(K+1:N,K) = A(K+1:N,K)/A(K,K)
!
! Row elimination performed by columns for efficiency
!
      DO J=K+1,N
         Pivot = A(Pivot_row,J)
         IF(Pivot_row /= K) THEN
!          Swap if pivot row is not K
           A(Pivot_row,J)=A(K,J)
           A(K,J)=Pivot
         ENDIF
         A(K+1:N,J)=A(K+1:N,J)-Pivot* A(K+1:N,K)
      END DO
!
! Apply same operations to B
!
      B(K+1:N)=B(K+1:N)-A(K+1:N,K)*B(K)
   END DO
!
! Backward substitution
!
   DO I=N,1,-1
      Sum = 0.0
      DO J= I+1,N
         Sum=Sum+A(I,J)*X(J)
      END DO
      X(I)=(B(I)-Sum)/A(I,I)
   END DO
END SUBROUTINE Gaussian_Elimination
```

24.7.1 Notes

24.7.1.1 Module for kind type

A module, Precisions, has been used to define a kind type parameter, Long, to specify the floating point precision to which we wish to work. This module is then used by the main program and the subroutine, and the kind type parameter Long is used with all the REAL type definitions and with any constants, e.g.,

```
REAL(Long), PARAMETER :: Eps=1.E-13_Long
```

24.7.1.2 Deferred-shape arrays

In the main program matrix A and vectors B and X are declared as deferred-shape arrays, by specifying their rank only and using the ALLOCATABLE attribute. Their shape is determined at run time when the variable N is read in and then the statement

```
ALLOCATE(A(1:N,1:N), B(1:N), X(1:N))
```

is used.

24.7.1.3 Intrinisic functions MAXVAL and MAXLOC

In the context of subroutine Gaussian_Elimination we have used:

```
MAXVAL ( MAXLOC (ABS ( A ( K:N,K ) ) ) ) + K - 1
```

Breaking this down,

```
MAXLOC ( ABS ( A (K:N,K) ) )
```

takes the rank 1 array

$$(|A(K,K)|,|A(K+1,K)|,\ldots|A(N,K)|) \qquad (1)$$

where $|A(K,K)| =$ ABS($A(K,K)$) and of length $N- K + 1$. It returns the position of the largest element as a rank 1 array of size one, e.g., (L)

Applying MAXVAL to this rank 1 array (L) returns L as a scalar, L being the position of the largest element of array (1).

What we actually want is the position of the largest element of (1) , but in the K^{th} column of matrix A. We therefore have to add $K-1$ to L to give the actual position in column K of A.

24.8 Notes on module usage and compilation

If we only have one file comprising all of the program units (main program, modules, functions and subroutines) then there is little to worry about. However, it is

recommended that larger-scale programs be developed as a collection of files with related program units in each file, or even one program unit per file. This is more productive in the longer term, but it will lead to problems with modules unless we compile each module **before** we use it in other program units.

Secondly, we must use one directory or subdirectory so that the compiler and linker can find each program unit.

Thirdly, we must be aware of the file naming conventions used by each compiler implementation we work with. Consider the following:

Fortran module name	Compaq under DOS	NAG f95 Sun Ultra Sparc
Precisions	Precisions.mod	Precisions.mod

Whilst in this case they are the same, this is not guaranteed.

24.9 Summary

We have now introduced the concept of a module, another type of program unit, probably one of of the most important features of Fortran 90. We have seen in this chapter how they can be used:

- Define global data.
- Define derived data types.
- Contain explicit procedure interfaces.
- Cackage together procedures.

This is a very powerful addition to the language, especially when constructing large programs and procedure libraries.

24.10 Problems

1. Write two functions, one to calculate the volume of a cylinder $\pi r^2 l$ where the radius is r and the length is l, and the other to calculate the area of the base of the cylinder πr^2. Define π as a parameter in a module which is used by the two functions. Now write a main program which prompts the user for the values of r and l, calls the two functions and prints out the results.

2. Make all the real variables in the above problem have 15 significant digits and a range of 10^{-307} to 10^{+307}. Use a module.

24.11 Bibliography

Dongarra, J., Bunch, J.R., Moler, C.B., and Stewart, G.W. *LINPACK User's Guide*. SIAM Publications, 1979.

- This Fortran 77 package is for the solution of simultaneous systems of linear algebraic equations. Special subroutines are included for many common types of coefficient matrices. The source is available through NETLIB. See Chapter 28 for more details.

Hopkins T., Phillips C., *Numerical Methods in Practice, using the NAG Library*. Addison-Wesley.

- This is a very good practical introduction to numerical analysis, with the aim of guiding users to the more commonly used routines in the NAG Fortran 77 library. It does this by introducing topics, giving some background, advantages and disadvantages, and the Fortran 77 code for some of the more well-known algorithms. It then introduces the appropriate NAG routine with a brief discussion of its use, calling sequence and any error reporting facilities. We've found this invaluable for many of our students who are users of the NAG library but not well versed with numerical analysis.
  Maybe we will see a Fortran 90 version of this book in the near future?

NAG. Visit their web site for up to date details of their products:

- http://www.nag.co.uk/

Visual Numerics. Visit their web site for details of their products:

- http://www.vni.com/index.html

25

Converting from Fortran 77

"Twas brillig, and the slithy toves
did gyre and gimble in the wabe;
All mimsy were the borogoves,
And the mome raths outgrabe."

Lewis Carroll

Aim

This chapter looks at some of the options available when working with older Fortran code.

25 Converting from Fortran 77

This chapter looks at converting Fortran 77 code to Fortran 90 and 95 styles.

The aim here is to provide the Fortran 77 programmer (and in particular the person with legacy code) with some simple guidelines for conversion.

The first thing that one must have is a thorough understanding of the newer, better language features of Fortran 95. It is essential that the material in the earlier chapters of this book be covered, and some of the problems attempted. This will provide a feel for Fortran 95.

The second thing one must have is a thorough understanding of the language constructs used in this legacy code. Use should be made of the compiler documentation for whatever Fortran 77 compiler you are using, as this will provide the detailed (often system specific) information required. The recommendations below are therefore brief.

It is possible to move gradually from Fortran 77 to Fortran 95. In many cases existing code can be quite simply recompiled by a suitable choice of compiler options. This enables us to mix and match old and new in one program. This process is likely to highlight nonstandard language features in your old code. There will inevitably be some problems here.

The first thing to consider is what the standard says. The standard identifies two kinds of decremented features; deleted and obsolescent. It is extremely unwise to consider the long-term use of these features as they are candidates for removal from future standards.

25.1 Deleted features

The list of deleted features for Fortran 95 is empty, i.e., there are none.

25.2 Obsolescent features

The obsolescent features are those for which better methods are available. They are given below with alternatives.

25.2.1 Arithmetic IF

Use the IF statement.

25.2.2 Real and double precision DO control variables

Use integer.

25.2.3 Shared DO termination and non-ENDDO termination

Use an END DO.

25.2.4 Alternate RETURN

Use a CASE statement on return. An error code has to be returned.

25.2.5 PAUSE statement

System specific. Normally easily replaced with a suitable READ statement.

25.2.6 ASSIGN and assigned GOTO statements

Fortunately rarely used.

25.2.7 Assigned FORMAT statements

Use character arrays, arrays and constants.

25.2.8 H editing

Use character edit descriptor.

25.3 Better alternatives

Below we are looking at the new features of the Fortran 95 standard, and how we can replace our current coding practices with the better facilities that now exist.

- DOUBLE PRECISION — use KIND, see Chapter 8, and examples throughout the book.
- fixed format — use free format
- implicit typing — use IMPLICIT NONE
- BLOCK DATA — use modules
- COMMON statement — use modules
- EQUIVALENCE — Invariably the use of this feature requires considerable system specific knowledge. There will be cases where there have been extremely good reasons why this feature has been used, normally efficiency related. However with the rapid changes taking place in the power and speed of hardware these reasons are diminishing.
- Assumed-size / explicit-shape dummy array arguments — If a dummy argument is assumed-size or explicit-shape (the only ones available in Fortran 77) then the ranks of the actual argument and the associated argument don't have to be the same. With Fortran 95 arrays are now objects instead of a linear sequence of elements, as was the case with Fortran 77, and now for array arguments the fundamental rule is that actual and dummy arguments have the same rank and same extents in each dimension, i.e., the same shape, and this is done using assumed-shape dummy array arguments. An interface block is mandatory for assumed-shape arrays.

- ENTRY statement — use module plus USE statement.
- Statement functions — use internal function, see Chapter 14.
- Computed GOTO — use CASE statement, see Chapter 15.
- Alternate RETURN — use error flags on calling routine.
- INCLUDE — use modules plus USE statement.
- EXTERNAL statement for dummy procedure arguments.

Use explicit interface blocks everywhere. This also provides argument checking and other benefits.

25.4 Example 1

The first and simplest option is to do nothing. Any code that is valid standard Fortran 77 will compile as the various successor standards require backwards compatibility with the Fortran 77 standard.

We will look at an example of leaving the Fortran 77 code alone using a sorting subroutine from netlib. To get hold of a copy of this code visit:

- http://www.netlib.org/

and search using

- sort

as the keyword.

One of the retrieved links should be

- http://www.netlib.org/slatec/src/dsort.f

Here is a complete listing of this subroutine as is. The code wraps in places at comment lines and this is intentional as we wanted to show you the code just as it is without any changes to fit the printed page

```
*DECK DSORT
       SUBROUTINE DSORT (DX, DY, N, KFLAG)
C***BEGIN PROLOGUE  DSORT
C***PURPOSE  Sort an array and optionally make the
same interchanges in
C               an auxiliary array.  The array may be
sorted in increasing
C               or decreasing order.  A slightly
modified QUICKSORT
C               algorithm is used.
```

```
C***LIBRARY    SLATEC
C***CATEGORY   N6A2B
C***TYPE       DOUBLE PRECISION (SSORT-S, DSORT-D,
ISORT-I)
C***KEYWORDS   SINGLETON QUICKSORT, SORT, SORTING
C***AUTHOR   Jones, R. E., (SNLA)
C              Wisniewski, J. A., (SNLA)
C***DESCRIPTION
C
C    DSORT sorts array DX and optionally makes the same
interchanges in
C    array DY.  The array DX may be sorted in
increasing order or
C    decreasing order.  A slightly modified quicksort
algorithm is used.
C
C    Description of Parameters
C       DX - array of values to be sorted    (usually
abscissas)
C       DY - array to be (optionally) carried along
C       N  - number of values in array DX to be sorted
C       KFLAG - control parameter
C               =  2  means sort DX in increasing order
and carry DY along.
C               =  1  means sort DX in increasing order
(ignoring DY)
C               = -1  means sort DX in decreasing order
(ignoring DY)
C               = -2  means sort DX in decreasing order
and carry DY along.
C
C***REFERENCES  R. C. Singleton, Algorithm 347, An
efficient algorithm
C                    for sorting with minimal storage,
Communications of
C                    the ACM, 12, 3 (1969), pp.
185-187.
C***ROUTINES CALLED  XERMSG
C***REVISION HISTORY  (YYMMDD)
C    761101  DATE WRITTEN
C    761118  Modified to use the Singleton quicksort
algorithm.  (JAW)
```

```
C    890531  Changed all specific intrinsics to
generic.  (WRB)
C    890831  Modified array declarations.  (WRB)
C    891009  Removed unreferenced statement labels.
(WRB)
C    891024  Changed category.  (WRB)
C    891024  REVISION DATE from Version 3.2
C    891214  Prologue converted to Version 4.0 format.
(BAB)
C    900315  CALLs to XERROR changed to CALLs to
XERMSG.  (THJ)
C    901012  Declared all variables; changed X,Y to
DX,DY; changed
C             code to parallel SSORT. (M. McClain)
C    920501  Reformatted the REFERENCES section.  (DWL,
WRB)
C    920519  Clarified error messages.  (DWL)
C    920801  Declarations section rebuilt and code
restructured to use
C             IF-THEN-ELSE-ENDIF.  (RWC, WRB)
C***END PROLOGUE  DSORT
C      .. Scalar Arguments ..
       INTEGER KFLAG, N
C      .. Array Arguments ..
       DOUBLE PRECISION DX(*), DY(*)
C      .. Local Scalars ..
       DOUBLE PRECISION R, T, TT, TTY, TY
       INTEGER I, IJ, J, K, KK, L, M, NN
C      .. Local Arrays ..
       INTEGER IL(21), IU(21)
C      .. External Subroutines ..
       EXTERNAL XERMSG
C      .. Intrinsic Functions ..
       INTRINSIC ABS, INT
C***FIRST EXECUTABLE STATEMENT  DSORT
       NN = N
       IF (NN .LT. 1) THEN
           CALL XERMSG ('SLATEC', 'DSORT',
     +       'The number of values to be sorted is
not positive.', 1, 1)
           RETURN
       ENDIF
```

```
C
       KK = ABS(KFLAG)
       IF (KK.NE.1 .AND. KK.NE.2) THEN
          CALL XERMSG ('SLATEC', 'DSORT',
     +       'The sort control parameter, K, is not 2,
1, -1, or -2.', 2,
     +       1)
          RETURN
       ENDIF
C
C      Alter array DX to get decreasing order if needed
C
       IF (KFLAG .LE. -1) THEN
          DO 10 I=1,NN
             DX(I) = -DX(I)
   10     CONTINUE
       ENDIF
C
       IF (KK .EQ. 2) GO TO 100
C
C      Sort DX only
C
       M = 1
       I = 1
       J = NN
       R = 0.375D0
C
   20  IF (I .EQ. J) GO TO 60
       IF (R .LE. 0.5898437D0) THEN
          R = R+3.90625D-2
       ELSE
          R = R-0.21875D0
       ENDIF
C
   30  K = I
C
C      Select a central element of the array and save
it in location T
C
       IJ = I + INT((J-I)*R)
       T = DX(IJ)
C
```

```
C      If first element of array is greater than T,
interchange with T
C
       IF (DX(I) .GT. T) THEN
          DX(IJ) = DX(I)
          DX(I) = T
          T = DX(IJ)
       ENDIF
       L = J
C
C      If last element of array is less than than T,
interchange with T
C
       IF (DX(J) .LT. T) THEN
          DX(IJ) = DX(J)
          DX(J) = T
          T = DX(IJ)
C
C         If first element of array is greater than T,
interchange with T
C
          IF (DX(I) .GT. T) THEN
             DX(IJ) = DX(I)
             DX(I) = T
             T = DX(IJ)
          ENDIF
       ENDIF
C
C      Find an element in the second half of the array
which is smaller
C      than T
C
   40 L = L-1
       IF (DX(L) .GT. T) GO TO 40
C
C      Find an element in the first half of the array
which is greater
C      than T
C
   50 K = K+1
       IF (DX(K) .LT. T) GO TO 50
C
```

```
C       Interchange these elements
C
        IF (K .LE. L) THEN
            TT = DX(L)
            DX(L) = DX(K)
            DX(K) = TT
            GO TO 40
        ENDIF
C
C       Save upper and lower subscripts of the array yet
to be sorted
C
        IF (L-I .GT. J-K) THEN
            IL(M) = I
            IU(M) = L
            I = K
            M = M+1
        ELSE
            IL(M) = K
            IU(M) = J
            J = L
            M = M+1
        ENDIF
        GO TO 70
C
C       Begin again on another portion of the unsorted
array
C
    60  M = M-1
        IF (M .EQ. 0) GO TO 190
        I = IL(M)
        J = IU(M)
C
    70  IF (J-I .GE. 1) GO TO 30
        IF (I .EQ. 1) GO TO 20
        I = I-1
C
    80  I = I+1
        IF (I .EQ. J) GO TO 60
        T = DX(I+1)
        IF (DX(I) .LE. T) GO TO 80
        K = I
```

```
C
    90 DX(K+1) = DX(K)
       K = K-1
       IF (T .LT. DX(K)) GO TO 90
       DX(K+1) = T
       GO TO 80
C
C      Sort DX and carry DY along
C
   100 M = 1
       I = 1
       J = NN
       R = 0.375D0
C
   110 IF (I .EQ. J) GO TO 150
       IF (R .LE. 0.5898437D0) THEN
           R = R+3.90625D-2
       ELSE
           R = R-0.21875D0
       ENDIF
C
   120 K = I
C
C      Select a central element of the array and save
it in location T
C
       IJ = I + INT((J-I)*R)
       T = DX(IJ)
       TY = DY(IJ)
C
C      If first element of array is greater than T,
interchange with T
C
       IF (DX(I) .GT. T) THEN
           DX(IJ) = DX(I)
           DX(I) = T
           T = DX(IJ)
           DY(IJ) = DY(I)
           DY(I) = TY
           TY = DY(IJ)
       ENDIF
       L = J
```

```
C
C      If last element of array is less than T,
interchange with T
C
       IF (DX(J) .LT. T) THEN
           DX(IJ) = DX(J)
           DX(J) = T
           T = DX(IJ)
           DY(IJ) = DY(J)
           DY(J) = TY
           TY = DY(IJ)
C
C          If first element of array is greater than T,
interchange with T
C
           IF (DX(I) .GT. T) THEN
               DX(IJ) = DX(I)
               DX(I) = T
               T = DX(IJ)
               DY(IJ) = DY(I)
               DY(I) = TY
               TY = DY(IJ)
           ENDIF
       ENDIF
C
C      Find an element in the second half of the array
which is smaller
C      than T
C
  130 L = L-1
       IF (DX(L) .GT. T) GO TO 130
C
C      Find an element in the first half of the array
which is greater
C      than T
C
  140 K = K+1
       IF (DX(K) .LT. T) GO TO 140
C
C      Interchange these elements
C
       IF (K .LE. L) THEN
```

```
            TT = DX(L)
            DX(L) = DX(K)
            DX(K) = TT
            TTY = DY(L)
            DY(L) = DY(K)
            DY(K) = TTY
            GO TO 130
         ENDIF
C
C      Save upper and lower subscripts of the array yet
to be sorted
C
         IF (L-I .GT. J-K) THEN
            IL(M) = I
            IU(M) = L
            I = K
            M = M+1
         ELSE
            IL(M) = K
            IU(M) = J
            J = L
            M = M+1
         ENDIF
         GO TO 160
C
C      Begin again on another portion of the unsorted
array
C
   150 M = M-1
         IF (M .EQ. 0) GO TO 190
         I = IL(M)
         J = IU(M)
C
   160 IF (J-I .GE. 1) GO TO 120
         IF (I .EQ. 1) GO TO 110
         I = I-1
C
   170 I = I+1
         IF (I .EQ. J) GO TO 150
         T = DX(I+1)
         TY = DY(I+1)
         IF (DX(I) .LE. T) GO TO 170
```

```
        K = I
C
   180 DX(K+1) = DX(K)
        DY(K+1) = DY(K)
        K = K-1
        IF (T .LT. DX(K)) GO TO 180
        DX(K+1) = T
        DY(K+1) = TY
        GO TO 170
C
C       Clean up
C
   190 IF (KFLAG .LE. -1) THEN
            DO 200 I=1,NN
                DX(I) = -DX(I)
   200      CONTINUE
        ENDIF
        RETURN
        END
```

Our aim is to replace a call to the Quicksort subroutine in an earlier example with a call to the dsort subroutine. The new program shall be called ch2501.f90 in what follows.

If we follow the Fortran 77 route all we need to do is change all DOUBLE PRECISION variables to REAL and comment out the calls to the external error handling subroutine XERMSG.

We then comment out the call to Quicksort:

```
! CALL quicksort(1,how_many)
```

and replace with

```
CALL DSORT(Raw_data,Raw_Data,How_many,1)
```

where the value of 1 for kflag means ignore the second array.

Here is an example of using the Intel compiler to compile and run the complete program:

- ifort -c dsort.f
- ifort ch2501.f90 dsort.obj
- ch2501

The first command compiles the dsort routine as a Fortran 77 fixed source form and generates an object file called dsort.obj.

The second command compiles the main program and modules and links this with the dsort.obj file.

The third line runs the program.

This example shows how easy it is in practice to mix and match both Fortran 77 and Fortran 90 style code.

Let us next look at converting the above dsort routine to Fortran 90/95.

25.5 Example 2

Mike Metcalf provides a free program to convert from Fortran 77 to Fortran 90 syntax. A copy can be found at

- http://www.kcl.ac.uk/fortran

Below is the output from running this program.

```
 Type name of file, shift, max. indent level, T or F
for blank treatment,
 T or F for interface blocks only.
 For simple use type only the name of the file
followed by a slash (/) and RETUR
N.
 Note that the name should be given WITHOUT extension!
dsort/
 Loop bodies will be indented by  0
 Maximum indenting level is        0
 Processing complete in    0.000 seconds
 Maximum depth of DO-loop nesting    1
 Maximum depth of IF-block nesting   2
 No. of lines read                  324
 No. of program units read            1
 Global syntax error flag             F
```

The program simply replaces the C in column 1 with the new comment symbol !. Here is what one needs to do to compile using the Intel compiler:

- ifort ch2501.f90 dsort.f90

This couldn't really be much simpler. Both methods are completely straightforward.

Other free conversions tools include

- http://www.owlnet.rice.edu/~colby/f2f.html

and here is a quote by the author about the software:

"f2f is a Perl script, which does much of the tedious work of converting Fortran 77 source code into Fortran 90/95 form. There seems to be a lot of Fortran-hate in the world, and I think this comes from people who have been forced to use Fortran 77 at some time or another. Hopefully, this program will make you a less hateful person."

25.6 Commercial conversion tools

There are a number of commercial conversion tools and some of them are given below.

25.6.1 NAG

Their home site is

- http://www.nag.co.uk/

Here is a Fortran 77 program with several subroutines and common blocks. The comments in the original program have been removed due to space considerations. The complete programs can be found at:

- http://www.kcl.ac.uk/fortran

The tsunami plot file can be found at

http://www.kcl.ac.uk/fortran

The program was written by Ian whilst on an 18-month secondment to the United Nations Environment Programme.

The code wraps in places and this is intentional as again we wanted to show you the code as it is without any changes to fit the printed page.

```
PROGRAM Map01
LOGICAL TRIAL,SCREEN
REAL LONG,LAT
SCREEN = .FALSE.
TRIAL = .FALSE.
CALL DATAIN(TRIAL)
PRINT *,' What resolution map do you want'
PRINT *
PRINT *,' 1 = 119,650'
PRINT *,' 2 =  75,500'
PRINT *,' 3 =  43,100'
PRINT *,' 4 =  19,300'
```

```
       PRINT *,' 5 =    4,420'
       PRINT *
  100 READ (UNIT=*,FMT=*,END=200,ERR=200) IRES
  200 IF ((IRES.LT.1) .OR. (IRES.GT.5)) THEN
           PRINT *,' Please input a number in the
range 1 to 5'
           GO TO 100
       END IF
       PRINT *,' What projection would you like?'
       PRINT *
       PRINT *,' 1 = Lambert         - equal area
-   rectangle'
       PRINT *,' 2 = Mercator        - equal direction
-   rectangle'
       PRINT *,' 3 = Hammer          - equal area
-   oval'
       PRINT *,' 4 = Bonne           -
-   heart'
       PRINT *,' 5 = Orthographic    - globe
-   round'
  300 READ (UNIT=*,FMT=*,END=400,ERR=400) IPROJ
  400 IF ((IPROJ.LT.1) .OR. (IPROJ.GT.5)) THEN
           PRINT *,' Please input a number in the
range 1 to 5'
           GO TO 300
       END IF
       LAT = 0.0
       LONG = 180.0
       PRINT *,' Which region do you wish to plot?'
       PRINT *,' 0 = all regions'
       PRINT *,' 1 = Hawaii'
       PRINT *,' 2 = New Zealand and South Pacific
Islands'
       PRINT *,' 3 = Papua New Guinea and Solomon
Islands'
       PRINT *,' 4 = Indonesia'
       PRINT *,' 5 = Philippines'
       PRINT *,' 6 = Japan'
       PRINT *,' 7 = Kuril Islands and Kamchatka'
       PRINT *,' 8 = Alaska incluing Aleutian Islands'
       PRINT *,' 9 = West Coast - North and Central
America'
```

```
       PRINT *,' 10 = West Coast - South America'
       READ (UNIT=*,FMT=*,END=8000,ERR=8000) NREG
 8000  IF ((NREG.LT.0) .OR. (NREG.GT.10)) THEN
            PRINT *,' Please input a number between 0
and 10 inclusive'
            GO TO 8000
       END IF
       PRINT *,' Which colour table do you wish to
use'
       PRINT *,' HLS = 1'
       PRINT *,' CMY = 2'
       PRINT *,' RGB = 3'
  500  READ (UNIT=*,FMT=*,END=600,ERR=600) ICOL
  600  IF ((ICOL.LT.1) .OR. (ICOL.GT.3)) THEN
            PRINT *,' Please input a number in the
range 1 to 3'
            GO TO 500
       END IF
       PRINT *,' Select device, a list of valid
devices maybe'
       PRINT *,' obtained by typing'
       PRINT *,' list *'
       PRINT *,' at the GROUTE prompt'
       CALL GROUTE(' ')
       CALL GOPEN
       CALL GSEGCR(1)
       CALL GSURFE
       IF (IRES.EQ.1) THEN
            CALL WEXTND
       ELSE IF (IRES.EQ.2) THEN
            CALL WRED1
       ELSE IF (IRES.EQ.3) THEN
            CALL WRED2
       ELSE IF (IRES.EQ.4) THEN
            CALL WRED3
       ELSE IF (IRES.EQ.5) THEN
            CALL WRED4
       END IF
       NR = 7
       KOLOR = 0
       CALL WOPEN(0,NR)
       CALL WPROJ(IPROJ)
```

```
        CALL WCENTR(LONG,LAT)
        CALL WDEFC(KOLOR)
        CALL WPLOT('     ',0.0)
        CALL CONVRT(TRIAL)
        CALL PLOTEM(TRIAL,NREG)
        CALL GSEGCR(1)
        CALL GCLOSE
        END
        SUBROUTINE DATAIN(TRIAL)
        LOGICAL TRIAL
        CHARACTER*80 FILNAM
        COMMON
/TSUNAM/REG0LA(378),REG0LO(378),REG1LA(206),REG1LO(206),
      +
REG2LA(41),REG2LO(41),REG3LA(54),REG3LO(54),REG4LA(60),
      +
REG4LO(60),REG5LA(1540),REG5LO(1540),REG6LA(80),REG6LO(8
0),
      +
REG7LA(144),REG7LO(144),REG8LA(245),REG8LO(245),
      +         REG9LA(285),REG9LO(285)

        IF (TRIAL.EQ..TRUE.) THEN
             PRINT *,' Entering data input phase'
        END IF
        FILNAM = 'tsunami.dat'
        OPEN (UNIT=50,FILE=FILNAM,ERR=30,STATUS='OLD')
        GO TO 40
   30 PRINT *,' Error opening data file'
        PRINT *,' Program terminates'
        STOP
   40 DO 100 I = 1,378
  100 READ (UNIT=50,FMT=1000) REG0LA(I),REG0LO(I)
 1000 FORMAT (1X,F7.2,2X,F7.2)
        DO 110 I = 1,206
  110 READ (UNIT=50,FMT=1000) REG1LA(I),REG1LO(I)
        DO 120 I = 1,41
  120 READ (UNIT=50,FMT=1000) REG2LA(I),REG2LO(I)
        DO 130 I = 1,54
  130 READ (UNIT=50,FMT=1000) REG3LA(I),REG3LO(I)
        DO 140 I = 1,60
  140 READ (UNIT=50,FMT=1000) REG4LA(I),REG4LO(I)
```

```
      DO 150 I = 1,1540
  150 READ (UNIT=50,FMT=1000) REG5LA(I),REG5LO(I)
      DO 160 I = 1,80
  160 READ (UNIT=50,FMT=1000) REG6LA(I),REG6LO(I)
      DO 170 I = 1,144
  170 READ (UNIT=50,FMT=1000) REG7LA(I),REG7LO(I)
      DO 180 I = 1,245
  180 READ (UNIT=50,FMT=1000) REG8LA(I),REG8LO(I)
      DO 190 I = 1,285
  190 READ (UNIT=50,FMT=1000) REG9LA(I),REG9LO(I)
      IF (TRIAL.EQ..TRUE.) THEN
          DO 200 I = 1,10
  200     PRINT *,REG0LA(I),'    ',REG0LO(I)
          PRINT *,' Exiting data input phase'
          READ *,DUMMY
      END IF
      END
      SUBROUTINE CONVRT(TRIAL)
      LOGICAL TRIAL
      COMMON
/TSUNAM/REG0LA(378),REG0LO(378),REG1LA(206),REG1LO(206),
     +
REG2LA(41),REG2LO(41),REG3LA(54),REG3LO(54),REG4LA(60),
     +
REG4LO(60),REG5LA(1540),REG5LO(1540),REG6LA(80),REG6LO(8
0),
     +
REG7LA(144),REG7LO(144),REG8LA(245),REG8LO(245),
     +        REG9LA(285),REG9LO(285)
      COMMON
/MMTSUN/MM0LA(378),MM0LO(378),MM1LA(206),MM1LO(206),
     +
MM2LA(41),MM2LO(41),MM3LA(54),MM3LO(54),MM4LA(60),
     +
MM4LO(60),MM5LA(1540),MM5LO(1540),MM6LA(80),MM6LO(80),
     +
MM7LA(144),MM7LO(144),MM8LA(245),MM8LO(245),MM9LA(285),
     +        MM9LO(285)

      IF (TRIAL.EQ..TRUE.) THEN
          PRINT *,' Entering convert'
      END IF
```

```
       DO 100 I = 1,378
  100 CALL
WGETMM(REG0LO(I),REG0LA(I),MM0LO(I),MM0LA(I))
       DO 110 I = 1,206
  110 CALL
WGETMM(REG1LO(I),REG1LA(I),MM1LO(I),MM1LA(I))
       DO 120 I = 1,41
  120 CALL
WGETMM(REG2LO(I),REG2LA(I),MM2LO(I),MM2LA(I))
       DO 130 I = 1,54
  130 CALL
WGETMM(REG3LO(I),REG3LA(I),MM3LO(I),MM3LA(I))
       DO 140 I = 1,60
  140 CALL
WGETMM(REG4LO(I),REG4LA(I),MM4LO(I),MM4LA(I))
       DO 150 I = 1,1540
  150 CALL
WGETMM(REG5LO(I),REG5LA(I),MM5LO(I),MM5LA(I))
       DO 160 I = 1,80
  160 CALL
WGETMM(REG6LO(I),REG6LA(I),MM6LO(I),MM6LA(I))
       DO 170 I = 1,144
  170 CALL
WGETMM(REG7LO(I),REG7LA(I),MM7LO(I),MM7LA(I))
       DO 180 I = 1,245
  180 CALL
WGETMM(REG8LO(I),REG8LA(I),MM8LO(I),MM8LA(I))
       DO 190 I = 1,285
  190 CALL
WGETMM(REG9LO(I),REG9LA(I),MM9LO(I),MM9LA(I))
       IF (TRIAL.EQ..TRUE.) THEN
            PRINT *,' Exiting convert'
       END IF
       END

       SUBROUTINE PLOTEM(TRIAL,NREG)
       LOGICAL TRIAL
       INTEGER NREG
       COMMON
/MMTSUN/MM0LA(378),MM0LO(378),MM1LA(206),MM1LO(206),
     +
MM2LA(41),MM2LO(41),MM3LA(54),MM3LO(54),MM4LA(60),
```

```
      +
MM4LO(60),MM5LA(1540),MM5LO(1540),MM6LA(80),MM6LO(80),
      +
MM7LA(144),MM7LO(144),MM8LA(245),MM8LO(245),MM9LA(285),
      +        MM9LO(285)
       DATA DWIDTH/1.0/

       IF (TRIAL.EQ..TRUE.) THEN
            DWIDTH = 5.0
            PRINT *,' Entering Plot points'
       END IF
       IF (NREG.EQ.0) THEN
            KOLOUR = 2
            CALL GWICOL(DWIDTH,KOLOUR)
            CALL GDOT(MM0LO,MM0LA,378)
            KOLOUR = 3
            CALL GWICOL(DWIDTH,KOLOUR)
            CALL GDOT(MM1LO,MM1LA,206)
            KOLOUR = 4
            CALL GWICOL(DWIDTH,KOLOUR)
            CALL GDOT(MM2LO,MM2LA,41)
            KOLOUR = 5
            CALL GWICOL(DWIDTH,KOLOUR)
            CALL GDOT(MM3LO,MM3LA,54)
            KOLOUR = 6
            CALL GWICOL(DWIDTH,KOLOUR)
            CALL GDOT(MM4LO,MM4LA,60)
            KOLOUR = 7
            CALL GWICOL(DWIDTH,KOLOUR)
            CALL GDOT(MM5LO,MM5LA,1540)
            KOLOUR = 0
            CALL GWICOL(DWIDTH,KOLOUR)
            CALL GDOT(MM6LO,MM6LA,80)
            KOLOUR = 24
            CALL GWICOL(DWIDTH,KOLOUR)
            CALL GDOT(MM7LO,MM7LA,144)
            KOLOUR = 23
            CALL GWICOL(DWIDTH,KOLOUR)
            CALL GDOT(MM8LO,MM8LA,245)
            KOLOUR = 22
            CALL GWICOL(DWIDTH,KOLOUR)
            CALL GDOT(MM9LO,MM9LA,285)
```

```
ELSE IF (NREG.EQ.1) THEN
     KOLOUR = 0
     CALL GWICOL(DWIDTH,KOLOUR)
     CALL GDOT(MM0LO,MM0LA,378)
ELSE IF (NREG.EQ.2) THEN
     KOLOUR = 2
     CALL GWICOL(DWIDTH,KOLOUR)
     CALL GDOT(MM1LO,MM1LA,206)
ELSE IF (NREG.EQ.3) THEN
     KOLOUR = 12
     CALL GWICOL(DWIDTH,KOLOUR)
     CALL GDOT(MM2LO,MM2LA,41)
ELSE IF (NREG.EQ.4) THEN
     KOLOUR = 4
     CALL GWICOL(DWIDTH,KOLOUR)
     CALL GDOT(MM3LO,MM3LA,54)
ELSE IF (NREG.EQ.5) THEN
     KOLOUR = 5
     CALL GWICOL(DWIDTH,KOLOUR)
     CALL GDOT(MM4LO,MM4LA,60)
ELSE IF (NREG.EQ.6) THEN
     KOLOUR = 6
     CALL GWICOL(DWIDTH,KOLOUR)
     CALL GDOT(MM5LO,MM5LA,1540)
ELSE IF (NREG.EQ.7) THEN
     KOLOUR = 7
     CALL GWICOL(DWIDTH,KOLOUR)
     CALL GDOT(MM6LO,MM6LA,80)
ELSE IF (NREG.EQ.8) THEN
     KOLOUR = 8
     CALL GWICOL(DWIDTH,KOLOUR)
     CALL GDOT(MM7LO,MM7LA,144)
ELSE IF (NREG.EQ.9) THEN
     KOLOUR = 9
     CALL GWICOL(DWIDTH,KOLOUR)
     CALL GDOT(MM8LO,MM8LA,245)
ELSE IF (NREG.EQ.10) THEN
     KOLOUR = 10
     CALL GWICOL(DWIDTH,KOLOUR)
     CALL GDOT(MM9LO,MM9LA,285)
END IF
IF (TRIAL.EQ..TRUE.) THEN
```

```
            PRINT *,' Exiting Plot points'
        END IF
        END
```

Below is the converted program after using the Nag tool suite. The code wraps in places and this is intentional as again we wanted to show you the code as it is without any changes to fit the printed page.

```
MODULE mmtsun

  INTEGER :: mm0la(378), mm0lo(378), mm1la(206),
mm1lo(206), mm2la(41), &
     mm2lo(41), mm3la(54), mm3lo(54), mm4la(60),
mm4lo(60), mm5la(1540), &
     mm5lo(1540), mm6la(80), mm6lo(80), mm7la(144),
mm7lo(144), mm8la(245), &
     mm8lo(245), mm9la(285), mm9lo(285)

END MODULE mmtsun
MODULE tsunam

  REAL :: reg0la(378), reg0lo(378), reg1la(206),
reg1lo(206), reg2la(41), &
     reg2lo(41), reg3la(54), reg3lo(54), reg4la(60),
reg4lo(60), reg5la(1540), &
     reg5lo(1540), reg6la(80), reg6lo(80), reg7la(144),
reg7lo(144), &
     reg8la(245), reg8lo(245), reg9la(285), reg9lo(285)

END MODULE tsunam
PROGRAM map01
! .. Local Scalars ..
  REAL :: lat, long
  INTEGER :: icol, iproj, ires, kolor, nr, nreg
  LOGICAL :: screen, trial
! ..
! .. External Subroutines ..
  EXTERNAL convrt, datain, gclose, gopen, groute,
gsegcr, gsurfe, plotem, &
     wcentr, wdefc, wextnd, wopen, wplot, wproj, wred1,
wred2, wred3, wred4
! ..
  screen = .FALSE.
```

```
   trial = .FALSE.
   CALL datain(trial)
   PRINT *, ' What resolution map do you want'
   PRINT *
   PRINT *, ' 1 = 119,650'
   PRINT *, ' 2 =  75,500'
   PRINT *, ' 3 =  43,100'
   PRINT *, ' 4 =  19,300'
   PRINT *, ' 5 =   4,420'
   PRINT *
100 READ (unit=*,fmt=*,end=200,err=200) ires
200 IF ((ires<1) .OR. (ires>5)) THEN
     PRINT *, ' Please input a number in the range 1
to 5'
     GO TO 100
   END IF
   PRINT *, ' What projection would you like?'
   PRINT *
   PRINT *, ' 1 = Lambert         - equal area
-  rectangle'
   PRINT *, ' 2 = Mercator        - equal direction    -
rectangle'
   PRINT *, ' 3 = Hammer          - equal area
-  oval'
   PRINT *, ' 4 = Bonne           -
-  heart'
   PRINT *, ' 5 = Orthographic   - globe               -
round'
300 READ (unit=*,fmt=*,end=400,err=400) iproj
400 IF ((iproj<1) .OR. (iproj>5)) THEN
     PRINT *, ' Please input a number in the range 1
to 5'
     GO TO 300
   END IF
   lat = 0.0
   long = 180.0
   PRINT *, ' Which region do you wish to plot?'
   PRINT *, ' 0 = all regions'
   PRINT *, ' 1 = Hawaii'
   PRINT *, ' 2 = New Zealand and South Pacific
Islands'
   PRINT *, ' 3 = Papua New Guinea and Solomon Islands'
```

```
   PRINT *, ' 4 = Indonesia'
   PRINT *, ' 5 = Philippines'
   PRINT *, ' 6 = Japan'
   PRINT *, ' 7 = Kuril Islands and Kamchatka'
   PRINT *, ' 8 = Alaska incluing Aleutian Islands'
   PRINT *, ' 9 = West Coast - North and Central
America'
   PRINT *, ' 10 = West Coast - South America'
   READ (unit=*,fmt=*,end=8000,err=8000) nreg
8000 IF ((nreg<0) .OR. (nreg>10)) THEN
     PRINT *, ' Please input a number between 0 and 10
inclusive'
     GO TO 8000
   END IF
   PRINT *, ' Which colour table do you wish to use'
   PRINT *, ' HLS = 1'
   PRINT *, ' CMY = 2'
   PRINT *, ' RGB = 3'
500 READ (unit=*,fmt=*,end=600,err=600) icol
600 IF ((icol<1) .OR. (icol>3)) THEN
     PRINT *, ' Please input a number in the range 1
to 3'
     GO TO 500
   END IF
   PRINT *, ' Select device, a list of valid devices
maybe'
   PRINT *, ' obtained by typing'
   PRINT *, ' list *'
   PRINT *, ' at the GROUTE prompt'
   CALL groute(' ')
   CALL gopen
   CALL gsegcr(1)
   CALL gsurfe
   IF (ires==1) THEN
     CALL wextnd
   ELSE IF (ires==2) THEN
     CALL wred1
   ELSE IF (ires==3) THEN
     CALL wred2
   ELSE IF (ires==4) THEN
     CALL wred3
   ELSE IF (ires==5) THEN
```

```
     CALL wred4
   END IF
   nr = 7
   kolor = 0
   CALL wopen(0,nr)
   CALL wproj(iproj)
   CALL wcentr(long,lat)
   CALL wdefc(kolor)
   CALL wplot('     ',0.0)
   CALL convrt(trial)
   CALL plotem(trial,nreg)
   CALL gsegcr(1)
   CALL gclose

END PROGRAM map01

SUBROUTINE datain(trial)

   USE tsunam , ONLY : reg0la, reg0lo, reg1la, reg1lo,
reg2la, reg2lo, reg3la, &
     reg3lo, reg4la, reg4lo, reg5la, reg5lo, reg6la,
reg6lo, reg7la, reg7lo, &
     reg8la, reg8lo, reg9la, reg9lo
! .. Scalar Arguments ..
   LOGICAL :: trial
! ..
! .. Local Scalars ..
   REAL :: dummy
   INTEGER :: i
   CHARACTER (80) :: filnam
! ..
! .. Arrays in Common ..
! ..
! .. Common Blocks ..
! ..
   IF (trial) THEN
     PRINT *, ' Entering data input phase'
   END IF
   filnam = 'tsunami.dat'
   OPEN (unit=50,file=filnam,err=30,status='OLD')
   GO TO 40
30 PRINT *, ' Error opening data file'
```

```
   PRINT *, ' Program terminates'
   STOP
40 DO 100 i = 1, 378
100 READ (unit=50,fmt=1000) reg0la(i), reg0lo(i)
1000 FORMAT (1X,F7.2,2X,F7.2)
   DO 110 i = 1, 206
110 READ (unit=50,fmt=1000) reg1la(i), reg1lo(i)
   DO 120 i = 1, 41
120 READ (unit=50,fmt=1000) reg2la(i), reg2lo(i)
   DO 130 i = 1, 54
130 READ (unit=50,fmt=1000) reg3la(i), reg3lo(i)
   DO 140 i = 1, 60
140 READ (unit=50,fmt=1000) reg4la(i), reg4lo(i)
   DO 150 i = 1, 1540
150 READ (unit=50,fmt=1000) reg5la(i), reg5lo(i)
   DO 160 i = 1, 80
160 READ (unit=50,fmt=1000) reg6la(i), reg6lo(i)
   DO 170 i = 1, 144
170 READ (unit=50,fmt=1000) reg7la(i), reg7lo(i)
   DO 180 i = 1, 245
180 READ (unit=50,fmt=1000) reg8la(i), reg8lo(i)
   DO 190 i = 1, 285
190 READ (unit=50,fmt=1000) reg9la(i), reg9lo(i)
   IF (trial) THEN
     DO 200 i = 1, 10
200 PRINT *, reg0la(i), '    ', reg0lo(i)
     PRINT *, ' Exiting data input phase'
     READ *, dummy
   END IF

END SUBROUTINE datain

SUBROUTINE convrt(trial)

   USE tsunam, ONLY : reg0la, reg0lo, reg1la, reg1lo,
reg2la, reg2lo, reg3la, &
     reg3lo, reg4la, reg4lo, reg5la, reg5lo, reg6la,
reg6lo, reg7la, reg7lo, &
     reg8la, reg8lo, reg9la, reg9lo
   USE mmtsun, ONLY : mm0la, mm0lo, mm1la, mm1lo,
mm2la, mm2lo, mm3la, mm3lo, &
```

```
     mm4la, mm4lo, mm5la, mm5lo, mm6la, mm6lo, mm7la,
mm7lo, mm8la, mm8lo, &
     mm9la, mm9lo
! .. Scalar Arguments ..
  LOGICAL :: trial
! ..
! .. Local Scalars ..
  INTEGER :: i
! ..
! .. External Subroutines ..
  EXTERNAL wgetmm
! ..
! .. Arrays in Common ..
! ..
! .. Common Blocks ..
! ..
  IF (trial) THEN
    PRINT *, ' Entering convert'
  END IF
  DO 100 i = 1, 378
100 CALL wgetmm(reg0lo(i),reg0la(i),mm0lo(i),mm0la(i))
  DO 110 i = 1, 206
110 CALL wgetmm(reg1lo(i),reg1la(i),mm1lo(i),mm1la(i))
  DO 120 i = 1, 41
120 CALL wgetmm(reg2lo(i),reg2la(i),mm2lo(i),mm2la(i))
  DO 130 i = 1, 54
130 CALL wgetmm(reg3lo(i),reg3la(i),mm3lo(i),mm3la(i))
  DO 140 i = 1, 60
140 CALL wgetmm(reg4lo(i),reg4la(i),mm4lo(i),mm4la(i))
  DO 150 i = 1, 1540
150 CALL wgetmm(reg5lo(i),reg5la(i),mm5lo(i),mm5la(i))
  DO 160 i = 1, 80
160 CALL wgetmm(reg6lo(i),reg6la(i),mm6lo(i),mm6la(i))
  DO 170 i = 1, 144
170 CALL wgetmm(reg7lo(i),reg7la(i),mm7lo(i),mm7la(i))
  DO 180 i = 1, 245
180 CALL wgetmm(reg8lo(i),reg8la(i),mm8lo(i),mm8la(i))
  DO 190 i = 1, 285
190 CALL wgetmm(reg9lo(i),reg9la(i),mm9lo(i),mm9la(i))
  IF (trial) THEN
    PRINT *, ' Exiting convert'
  END IF
```

```
END SUBROUTINE convrt

SUBROUTINE plotem(trial,nreg)

  USE mmtsun, ONLY : mm0la, mm0lo, mm1la, mm1lo,
mm2la, mm2lo, mm3la, mm3lo, &
     mm4la, mm4lo, mm5la, mm5lo, mm6la, mm6lo, mm7la,
mm7lo, mm8la, mm8lo, &
     mm9la, mm9lo
! .. Scalar Arguments ..
  INTEGER :: nreg
  LOGICAL :: trial
! ..
! .. Local Scalars ..
  REAL :: dwidth
  INTEGER :: kolour
! ..
! .. External Subroutines ..
  EXTERNAL gdot, gwicol
! ..
! .. Arrays in Common ..
! ..
! .. Common Blocks ..
! ..
! .. Data Statements ..
  DATA dwidth/1.0/
! ..
  IF (trial) THEN
    dwidth = 5.0
    PRINT *, ' Entering Plot points'
  END IF
  IF (nreg==0) THEN
    kolour = 2
    CALL gwicol(dwidth,kolour)
    CALL gdot(mm0lo,mm0la,378)
    kolour = 3
    CALL gwicol(dwidth,kolour)
    CALL gdot(mm1lo,mm1la,206)
    kolour = 4
    CALL gwicol(dwidth,kolour)
    CALL gdot(mm2lo,mm2la,41)
```

```
    kolour = 5
    CALL gwicol(dwidth,kolour)
    CALL gdot(mm3lo,mm3la,54)
    kolour = 6
    CALL gwicol(dwidth,kolour)
    CALL gdot(mm4lo,mm4la,60)
    kolour = 7
    CALL gwicol(dwidth,kolour)
    CALL gdot(mm5lo,mm5la,1540)
    kolour = 0
    CALL gwicol(dwidth,kolour)
    CALL gdot(mm6lo,mm6la,80)
    kolour = 24
    CALL gwicol(dwidth,kolour)
    CALL gdot(mm7lo,mm7la,144)
    kolour = 23
    CALL gwicol(dwidth,kolour)
    CALL gdot(mm8lo,mm8la,245)
    kolour = 22
    CALL gwicol(dwidth,kolour)
    CALL gdot(mm9lo,mm9la,285)
  ELSE IF (nreg==1) THEN
    kolour = 0
    CALL gwicol(dwidth,kolour)
    CALL gdot(mm0lo,mm0la,378)
  ELSE IF (nreg==2) THEN
    kolour = 2
    CALL gwicol(dwidth,kolour)
    CALL gdot(mm1lo,mm1la,206)
  ELSE IF (nreg==3) THEN
    kolour = 12
    CALL gwicol(dwidth,kolour)
    CALL gdot(mm2lo,mm2la,41)
  ELSE IF (nreg==4) THEN
    kolour = 4
    CALL gwicol(dwidth,kolour)
    CALL gdot(mm3lo,mm3la,54)
  ELSE IF (nreg==5) THEN
    kolour = 5
    CALL gwicol(dwidth,kolour)
    CALL gdot(mm4lo,mm4la,60)
  ELSE IF (nreg==6) THEN
```

```
      kolour = 6
      CALL gwicol(dwidth,kolour)
      CALL gdot(mm5lo,mm5la,1540)
   ELSE IF (nreg==7) THEN
      kolour = 7
      CALL gwicol(dwidth,kolour)
      CALL gdot(mm6lo,mm6la,80)
   ELSE IF (nreg==8) THEN
      kolour = 8
      CALL gwicol(dwidth,kolour)
      CALL gdot(mm7lo,mm7la,144)
   ELSE IF (nreg==9) THEN
      kolour = 9
      CALL gwicol(dwidth,kolour)
      CALL gdot(mm8lo,mm8la,245)
   ELSE IF (nreg==10) THEN
      kolour = 10
      CALL gwicol(dwidth,kolour)
      CALL gdot(mm9lo,mm9la,285)
   END IF
   IF (trial) THEN
      PRINT *, ' Exiting Plot points'
   END IF

END SUBROUTINE plotem
```

Some of the key points include:

- Generation of modules from common blocks.
- Generation of USE statements with the ONLY option to explicitly specify which variables are going to be made available in a particular subroutine.
- Documenting of variable, intrinsic and external usage within a subroutine.
- Code restructuring into a well laid out style.

The Nag tool suite can obviously be used to help maintain code during development.

25.6.2 Polyhedron

Their home site is

- http://www.polyhedron.com/

and the conversion of dsort.f is given below.

The code wraps in places and this is intentional as again we wanted to show you the code as it is without any changes to fit the printed page.

```
!*==DSORT.f90  processed by SPAG 6.55Dc at 17:45 on  4
May 2005
!*------------------    SPAG Configuration Options
--------------------
!*--0233,12 021101,-1
000000100000031111000002000020110201210,72 111 --
!*--1000000000121141100000000000,100,50,20,10 52,99000
12000000000031 --
!*--99011000000000000,72,72 02,42,38,33
000110121100001000000000       --
!*--------------------------------------------------------
----------------
!DECK DSORT
SUBROUTINE DSORT(Dx,Dy,N,Kflag)
IMPLICIT NONE
!*--DSORT10
!***BEGIN PROLOGUE  DSORT
!***PURPOSE  Sort an array and optionally make the
same interchanges in
!               an auxiliary array.  The array may be
sorted in increasing
!               or decreasing order.  A slightly
modified QUICKSORT
!               algorithm is used.
!***LIBRARY    SLATEC
!***CATEGORY   N6A2B
!***TYPE        REAL (SSORT-S, DSORT-D, ISORT-I)
!***KEYWORDS   SINGLETON QUICKSORT, SORT, SORTING
!***AUTHOR  Jones, R. E., (SNLA)
!             Wisniewski, J. A., (SNLA)
!***DESCRIPTION
!
!    DSORT sorts array DX and optionally makes the same
interchanges in
!    array DY.  The array DX may be sorted in
increasing order or
!    decreasing order.  A slightly modified quicksort
algorithm is used.
!
!    Description of Parameters
```

```
!       DX - array of values to be sorted   (usually
abscissas)
!       DY - array to be (optionally) carried along
!       N  - number of values in array DX to be sorted
!       KFLAG - control parameter
!             =  2  means sort DX in increasing order
and carry DY along.
!             =  1  means sort DX in increasing order
(ignoring DY)
!             = -1  means sort DX in decreasing order
(ignoring DY)
!             = -2  means sort DX in decreasing order
and carry DY along.
!
!***REFERENCES  R. C. Singleton, Algorithm 347, An
efficient algorithm
!                    for sorting with minimal storage,
Communications of
!                    the ACM, 12, 3 (1969), pp.
185-187.
!***ROUTINES CALLED  XERMSG
!***REVISION HISTORY  (YYMMDD)
!    761101  DATE WRITTEN
!    761118  Modified to use the Singleton quicksort
algorithm.  (JAW)
!    890531  Changed all specific intrinsics to
generic.  (WRB)
!    890831  Modified array declarations.  (WRB)
!    891009  Removed unreferenced statement labels.
(WRB)
!    891024  Changed category.  (WRB)
!    891024  REVISION DATE from Version 3.2
!    891214  Prologue converted to Version 4.0 format.
(BAB)
!    900315  CALLs to XERROR changed to CALLs to
XERMSG.  (THJ)
!    901012  Declared all variables; changed X,Y to
DX,DY; changed
!             code to parallel SSORT. (M. McClain)
!    920501  Reformatted the REFERENCES section.  (DWL,
WRB)
!    920519  Clarified error messages.  (DWL)
```

```
!    920801  Declarations section rebuilt and code
restructured to use
!              IF-THEN-ELSE-ENDIF.   (RWC, WRB)
!***END PROLOGUE  DSORT
!      .. Scalar Arguments ..
INTEGER Kflag , N
!      .. Array Arguments ..
REAL Dx(*) , Dy(*)
!      .. Local Scalars ..
REAL r , t , tt , tty , ty
INTEGER i , ij , j , k , kk , l , m , nn
!      .. Local Arrays ..
INTEGER il(21) , iu(21)
!      .. External Subroutines ..
!       EXTERNAL XERMSG
!      .. Intrinsic Functions ..
INTRINSIC ABS , INT
  CALL
SB$ENT('DSORT','D:\document\f2003\examples\ch25\polyhedr
on\dsort.f'&
  & )
!***FIRST EXECUTABLE STATEMENT  DSORT
  CALL BL$ENT(65)
  nn = N
  IF ( nn<1 ) THEN
!           CALL XERMSG ('SLATEC', 'DSORT',
!      +       'The number of values to be sorted is
not positive.', 1, 1)
    CALL BL$ENT(69)
    CALL SB$EXI
    RETURN
  ENDIF
!
  CALL BL$ENT(72)
  kk = ABS(Kflag)
  IF ( kk/=1 .AND. kk/=2 ) THEN
!           CALL XERMSG ('SLATEC', 'DSORT',
!      +       'The sort control parameter, K, is not
2, 1, -1, or -2.', 2,
!      +       1)
    CALL BL$ENT(77)
    CALL SB$EXI
```

```
    RETURN
   ENDIF
!
!      Alter array DX to get decreasing order if needed
!
   CALL BL$ENT(82)
   IF ( Kflag<=-1 ) THEN
    CALL BL$ENT(83)
    DO i = 1 , nn
      CALL BL$ENT(84)
      Dx(i) = -Dx(i)
    ENDDO
   ENDIF
!
   CALL BL$ENT(88)
   IF ( kk==2 ) GOTO 900
!
!      Sort DX only
!
   CALL BL$ENT(92)
   m = 1
   i = 1
   j = nn
   r = 0.375D0
!
    100  CALL BL$ENT(97)
         IF ( i==j ) GOTO 500
   CALL BL$ENT(98)
   IF ( r<=0.5898437D0 ) THEN
    CALL BL$ENT(99)
    r = r + 3.90625D-2
   ELSE
    CALL BL$ENT(101)
    r = r - 0.21875D0
   ENDIF
!
    200  CALL BL$ENT(104)
         k = i
!
!      Select a central element of the array and save
it in location T
!
```

```
   ij = i + INT((j-i)*r)
   t = Dx(ij)
!
!      If first element of array is greater than T,
interchange with T
!
   IF ( Dx(i)>t ) THEN
    CALL BL$ENT(114)
    Dx(ij) = Dx(i)
    Dx(i) = t
    t = Dx(ij)
   ENDIF
   CALL BL$ENT(118)
   l = j
!
!      If last element of array is less than than T,
interchange with T
!
   IF ( Dx(j)<t ) THEN
    CALL BL$ENT(123)
    Dx(ij) = Dx(j)
    Dx(j) = t
    t = Dx(ij)
!
!          If first element of array is greater than T,
interchange with T
!
    IF ( Dx(i)>t ) THEN
      CALL BL$ENT(130)
      Dx(ij) = Dx(i)
      Dx(i) = t
      t = Dx(ij)
    ENDIF
   ENDIF
!
!      Find an element in the second half of the array
which is smaller
!      than T
!
    300  CALL BL$ENT(139)
         l = l - 1
   IF ( Dx(l)>t ) GOTO 300
```

```
!
!      Find an element in the first half of the array
which is greater
!      than T
!
    400  CALL BL$ENT(145)
         k = k + 1
   IF ( Dx(k)<t ) GOTO 400
!
!      Interchange these elements
!
   CALL BL$ENT(150)
   IF ( k<=l ) THEN
    CALL BL$ENT(151)
    tt = Dx(l)
    Dx(l) = Dx(k)
    Dx(k) = tt
    GOTO 300
   ENDIF
!
!      Save upper and lower subscripts of the array yet
to be sorted
!
   CALL BL$ENT(159)
   IF ( l-i>j-k ) THEN
    CALL BL$ENT(160)
    il(m) = i
    iu(m) = l
    i = k
    m = m + 1
   ELSE
    CALL BL$ENT(165)
    il(m) = k
    iu(m) = j
    j = l
    m = m + 1
   ENDIF
   CALL BL$ENT(170)
   GOTO 600
!
!      Begin again on another portion of the unsorted
array
```

```
!
    500  CALL BL$ENT(174)
         m = m - 1
   IF ( m==0 ) GOTO 1800
   CALL BL$ENT(176)
   i = il(m)
   j = iu(m)
!
    600  CALL BL$ENT(179)
         IF ( j-i>=1 ) GOTO 200
   CALL BL$ENT(180)
   IF ( i==1 ) GOTO 100
   CALL BL$ENT(181)
   i = i - 1
!
    700  CALL BL$ENT(183)
         i = i + 1
   IF ( i==j ) GOTO 500
   CALL BL$ENT(185)
   t = Dx(i+1)
   IF ( Dx(i)<=t ) GOTO 700
   CALL BL$ENT(187)
   k = i
!
    800  CALL BL$ENT(189)
         Dx(k+1) = Dx(k)
   k = k - 1
   IF ( t<Dx(k) ) GOTO 800
   CALL BL$ENT(192)
   Dx(k+1) = t
   GOTO 700
!
!      Sort DX and carry DY along
!
    900  CALL BL$ENT(197)
         m = 1
   i = 1
   j = nn
   r = 0.375D0
!
    1000 CALL BL$ENT(202)
         IF ( i==j ) GOTO 1400
```

```
   CALL BL$ENT(203)
   IF ( r<=0.5898437D0 ) THEN
    CALL BL$ENT(204)
    r = r + 3.90625D-2
   ELSE
    CALL BL$ENT(206)
    r = r - 0.21875D0
   ENDIF
!
    1100 CALL BL$ENT(209)
         k = i
!
!      Select a central element of the array and save
it in location T
!
   ij = i + INT((j-i)*r)
   t = Dx(ij)
   ty = Dy(ij)
!
!      If first element of array is greater than T,
interchange with T
!
   IF ( Dx(i)>t ) THEN
    CALL BL$ENT(220)
    Dx(ij) = Dx(i)
    Dx(i) = t
    t = Dx(ij)
    Dy(ij) = Dy(i)
    Dy(i) = ty
    ty = Dy(ij)
   ENDIF
   CALL BL$ENT(227)
   l = j
!
!      If last element of array is less than T,
interchange with T
!
   IF ( Dx(j)<t ) THEN
    CALL BL$ENT(232)
    Dx(ij) = Dx(j)
    Dx(j) = t
    t = Dx(ij)
```

```
    Dy(ij) = Dy(j)
    Dy(j) = ty
    ty = Dy(ij)
!
!          If first element of array is greater than T,
interchange with T
!
    IF ( Dx(i)>t ) THEN
      CALL BL$ENT(242)
      Dx(ij) = Dx(i)
      Dx(i) = t
      t = Dx(ij)
      Dy(ij) = Dy(i)
      Dy(i) = ty
      ty = Dy(ij)
    ENDIF
   ENDIF
!
!      Find an element in the second half of the array
which is smaller
!      than T
!
    1200 CALL BL$ENT(254)
         l = l - 1
   IF ( Dx(l)>t ) GOTO 1200
!
!      Find an element in the first half of the array
which is greater
!      than T
!
    1300 CALL BL$ENT(260)
         k = k + 1
   IF ( Dx(k)<t ) GOTO 1300
!
!      Interchange these elements
!
   CALL BL$ENT(265)
   IF ( k<=l ) THEN
    CALL BL$ENT(266)
    tt = Dx(l)
    Dx(l) = Dx(k)
    Dx(k) = tt
```

```
    tty = Dy(l)
    Dy(l) = Dy(k)
    Dy(k) = tty
    GOTO 1200
   ENDIF
!
!      Save upper and lower subscripts of the array yet
to be sorted
!
   CALL BL$ENT(277)
   IF ( l-i>j-k ) THEN
    CALL BL$ENT(278)
    il(m) = i
    iu(m) = l
    i = k
    m = m + 1
   ELSE
    CALL BL$ENT(283)
    il(m) = k
    iu(m) = j
    j = l
    m = m + 1
   ENDIF
   CALL BL$ENT(288)
   GOTO 1500
!
!      Begin again on another portion of the unsorted
array
!
    1400 CALL BL$ENT(292)
         m = m - 1
   IF ( m==0 ) GOTO 1800
   CALL BL$ENT(294)
   i = il(m)
   j = iu(m)
!
    1500 CALL BL$ENT(297)
         IF ( j-i>=1 ) GOTO 1100
   CALL BL$ENT(298)
   IF ( i==1 ) GOTO 1000
   CALL BL$ENT(299)
   i = i - 1
```

```
!
    1600 CALL BL$ENT(301)
         i = i + 1
   IF ( i==j ) GOTO 1400
   CALL BL$ENT(303)
   t = Dx(i+1)
   ty = Dy(i+1)
   IF ( Dx(i)<=t ) GOTO 1600
   CALL BL$ENT(306)
   k = i
!
    1700 CALL BL$ENT(308)
         Dx(k+1) = Dx(k)
   Dy(k+1) = Dy(k)
   k = k - 1
   IF ( t<Dx(k) ) GOTO 1700
   CALL BL$ENT(312)
   Dx(k+1) = t
   Dy(k+1) = ty
   GOTO 1600
!
!      Clean up
!
    1800 CALL BL$ENT(318)
         IF ( Kflag<=-1 ) THEN
    CALL BL$ENT(319)
    DO i = 1 , nn
      CALL BL$ENT(320)
      Dx(i) = -Dx(i)
    ENDDO
   ENDIF
   CALL BL$ENT(323)
   CONTINUE
   CALL SB$EXI
   END SUBROUTINE DSORT
```

Changing the subroutine using an editor would obviously be much more tedious and error prone.

Below is an example from their site that looks at the same subroutine in Fortran 66, 77 and 90 styles.

25.6.3 Original Fortran 66

This subroutine picks off digits from an integer and branches depending on their value.

```
      SUBROUTINE OBACT(TODO)
      INTEGER TODO,DONE,IP,BASE
      COMMON /EG1/N,L,DONE
      PARAMETER (BASE=10)
   13 IF(TODO.EQ.0) GO TO 12
      I=MOD(TODO,BASE)
      TODO=TODO/BASE
      GO TO(62,42,43,62,404,45,62,62,62),I
      GO TO 13
   42 CALL COPY
      GO TO 127
   43 CALL MOVE
      GO TO 144
  404 N=-N
   44 CALL DELETE
      GO TO 127
   45 CALL PRINT
      GO TO 144
   62 CALL BADACT(I)
      GO TO 12
  127 L=L+N
  144 DONE=DONE+1
      CALL RESYNC
      GO TO 13
   12 RETURN
      END
```

25.6.4 Fortran 77 Version

In addition to restructuring, SPAG has renamed some variables, removed the unused variable IP, inserted declarations, and used upper and lower case to distinguish different types of variable:

```
      SUBROUTINE OBACT(Todo)
      IMPLICIT NONE
C*** Start of declarations inserted by SPAG
      INTEGER act , LENgth , NCHar
C*** End of declarations inserted by SPAG
      INTEGER Todo , DONe , BASE
      COMMON /EG1   / NCHar , LENgth , DONe
```

```
       PARAMETER (BASE=10)
 100   IF ( Todo.NE.0 ) THEN
           act = MOD(Todo,BASE)
           Todo = Todo/BASE
           IF ( act.EQ.1 .OR. act.EQ.4 .OR.
      &          act.EQ.7 .OR. act.EQ.8 .OR.
      &          act.EQ.9 ) THEN
               CALL BADACT(act)
               GOTO 200
           ELSEIF ( act.EQ.2 ) THEN
               CALL COPY
               LENgth = LENgth + NCHar
           ELSEIF ( act.EQ.3 ) THEN
               CALL MOVE
           ELSEIF ( act.EQ.5 ) THEN
               NCHar = -NCHar
               CALL DELETE
               LENgth = LENgth + NCHar
           ELSEIF ( act.EQ.6 ) THEN
               CALL PRINT
           ELSE
               GOTO 100
           ENDIF
           DONe = DONe + 1
           CALL RESYNC
           GOTO 100
       ENDIF
 200   RETURN
       END
```

25.6.5 Fortran 90 Version

SPAG has used DO WHILE, SELECT CASE, EXIT and CYCLE. No GOTOs or labels remain.

```
       SUBROUTINE OBACT(Todo)
       IMPLICIT NONE
C*** Start of declarations inserted by SPAG
       INTEGER act , LENgth , NCHar
C*** End of declarations inserted by SPAG
       INTEGER Todo , DONe , BASE
       COMMON /EG1   / NCHar , LENgth , DONe
       PARAMETER (BASE=10)
       DO WHILE ( Todo.NE.0 )
```

```
        act = MOD(Todo,BASE)
        Todo = Todo/BASE
        SELECT CASE (act)
        CASE (1,4,7,8,9)
            CALL BADACT(act)
            EXIT
        CASE (2)
            CALL COPY
            LENgth = LENgth + NCHar
        CASE (3)
            CALL MOVE
        CASE (5)
            NCHar = -NCHar
            CALL DELETE
            LENgth = LENgth + NCHar
        CASE (6)
            CALL PRINT
        CASE DEFAULT
            CYCLE
        END SELECT
        DONe = DONe + 1
        CALL RESYNC
    ENDDO
    RETURN
    END
```

This tool suite can also be used in the maintenance of code during development.

25.7 Summary

This chapter has shown some of the options open to you when working with legacy code. The emphasis has been on relatively straightforward code restructuring. The use of software tools to aid in this is highly recommended as converting manually using an editor is obviously going to involve much more work.

In Chapter 26 we will look at an example that involves a major rewrite using user defined data types.

25.8 Problems

1. Try out example 1 with your compiler. What compiler and linker options did you need?

2. Get hold of the Metcalf conversion program and try example 2. What compiler options did you need?

26

Case Studies

"The good teacher is a guide who helps others to dispense with his services."

R. S. Peters, *Ethics and Education*

Aims

The aims of this chapter are to look at several complete examples highlighting a variety of aspects of the use of Fortran 95:

- Using linked lists for sparse matrix problems.
- The solution of a set of ordinary differential equations using the Runga–Kutta–Merson method, with the use of a procedure as a parameter, and the use of work arrays.
- Generic procedures.
- A function that returns a variable length array.
- Operator and assignment overloading.
- Diagonal extraction of a matrix.
- Modules and packaging.
- Pure and elemental functions.
- Elemental subroutines.

26 Case Studies

This chapter looks at more realistic case studies of the use of Fortran 95 and its new features. There are examples of:

- Using linked lists for sparse matrix problems.
- The solution of a set of ordinary differential equations using the Runga–Kutta–Merson method, with the use of a procedure as a parameter, and the use of work arrays.
- The construction of generic procedures in Fortran 95. Many of the internal functions will take arguments of a variety of data types and return a result of the same type e.g., SINE will take an integer argument, real argument of whatever precision, complex argument and return the appropriate result.
- Operator and assignment overloading and the use of a MODULE PROCEDURE.
- The extraction of the diagonal elements of a matrix.
- Pure and elemental functions.
- Elemental subroutines.

The examples have been chosen to highlight the better features of Fortran 95 and what is possible with a modern language.

26.1 Using linked lists for sparse matrix problems

A matrix is said to be sparse if many of its elements are zero. Mathematical models in areas such as management science, power systems analysis, circuit theory and structural analysis consist of very large sparse systems of linear equations. It is not possible to solve these systems with classical methods because the sparsity would be lost and the eventual system would become too large to solve. Many of these systems consist of tens of thousands, hundreds of thousands and millions of equations. As computer systems become ever more powerful with massive amounts of memory the solution of even larger problems becomes feasible.

Direct Methods for Sparse Matrices, by Duff I.S., Erismon A.M. and Reid J.K., looks at direct methods for solving sparse systems of linear equations.

Sparse matrix techniques lend themselves to the use of dynamic data structures in Fortran 95. Only the nonzero elements of a sparse matrix need be stored, together with their positions in the matrix. Other information also needs to be stored so that row or column manipulation can be performed without repeated scanning of a potentially very large data structure. Sparse methods may involve introducing some new nonzero elements, and a way is needed of inserting them into the data struc-

ture. This is where the Fortran 95 pointer construct can be used. The sparse matrix can be implemented using a linked list to which entries can be easily added and from which they can be easily deleted.

As a simple introduction, consider the storage of sparse vectors. What we learn here can easily be applied to sparse matrices, which can be thought of as sets of sparse vectors.

26.1.1 Inner product of two sparse vectors

Assume that we have two sparse vectors x and y, for example:

$$\underline{x} = \begin{bmatrix} 3 \\ 0 \\ 5 \\ 0 \\ 0 \\ 4 \end{bmatrix} \qquad \underline{y} = \begin{bmatrix} 0 \\ 1 \\ 3 \\ 0 \\ 2 \\ 1 \end{bmatrix}$$

and we wish to calculate the inner product $x^T \; y \equiv \sum_{i=1}^{n} \; x_i \; \; y_i$. There are a number of approaches to doing this and the one we use in the program below stores them as two linked lists. Only the nonzero elements are stored (together with their indices):

```
   x data file       y data file
      3  1              1  2
      5  3              3  3
      4  6              2  5
                        1  6
```

```
PROGRAM ch2601
!
! This program reads the non-zero elements of
! two sparse vectors x and y together with their
! indices, and stores them in two linked lists.
! Using these linked lists it then calculates
! and prints out the inner product.
! It also prints the values.
!
! updated 21/3/00 to initialise pointers to
! be disassociated using intrinsic function NULL
! plus minor updates
!
```

```
   IMPLICIT NONE
   CHARACTER (LEN=30):: Filename
   TYPE sparse_vector
   INTEGER :: index
   REAL:: value
   TYPE (sparse_vector), POINTER ::next=> NULL ( )
   END TYPE sparse_vector
   TYPE(sparse_vector), POINTER ::    Root_x,Current_x, &
                        Root_y,Current_y
   REAL :: Inner_prod=0.0
   INTEGER::IO_status
!
! Read non-zero elements of vector x together
! with indices into a linked list
!
   PRINT *,'input file name for vector x'
   READ '(A)',Filename
   OPEN(UNIT=1 , FILE=Filename , STATUS='OLD' &
   , IOSTAT=IO_status)
   IF(IO_status /= 0)THEN
      PRINT*,'Error opening file ',Filename
      STOP
   ENDIF
   ALLOCATE(Root_x)
   READ (UNIT=1 , FMT=* , IOSTAT=IO_status) &
      Root_x%value,Root_x%index
   IF(IO_status /= 0) THEN
      PRINT*,' Error when reading from file ' &
      , Filename, ' or file empty'
      STOP
   ENDIF
!
! Read data for vector x from file until eof
!
   Current_x => Root_x
   ALLOCATE(Current_x%next)
   DO WHILE(ASSOCIATED(Current_x%next))
      Current_x => Current_x%next
      READ (UNIT=1,FMT=*,IOSTAT=IO_status) &
         Current_x%value, Current_x%index
      IF(IO_status == 0)THEN
         ALLOCATE(Current_x%next)
```

```
        CYCLE
      ELSEIF(IO_status > 0 )THEN
!
! Error on reading
!
        PRINT * ,'Error occurred when reading from ' &
                , Filename
        STOP
      ELSE
!
! End of file
!
        NULLIFY (Current_x%next)
      END IF
    END DO

    CLOSE(UNIT=1)
!
! Read non-zero elements of vector y together
! with indices into a linked list
!
    PRINT *,'input file name for vector y'
    READ '(A)',Filename
    OPEN(UNIT=1 , FILE=Filename , STATUS='OLD' &
     , IOSTAT=IO_status)
    IF(IO_status /= 0)THEN
      PRINT*,'Error opening file ',Filename
      STOP
    ENDIF
    ALLOCATE(Root_y)
    READ (UNIT=1 , FMT=* , IOSTAT=IO_status) &
       Root_y%value,Root_y%index
    IF(IO_status /= 0) THEN
      PRINT*,' Error when reading from ' &
        , Filename, ' or file empty'
      STOP
    ENDIF
!
! Read data for vector y from file until eof
!
    Current_y => Root_y
    ALLOCATE(Current_y%next)
```

```
   DO WHILE(ASSOCIATED(Current_y%next))
      Current_y => Current_y%next
      READ (UNIT=1 , FMT=* , IOSTAT=IO_status) &
        Current_y%value, Current_y%index
      IF(IO_status == 0)THEN
        ALLOCATE(Current_y%next)
        CYCLE
      ELSEIF(IO_status > 0 )THEN
!
! Error on reading
!
        PRINT * , 'Error occurred when reading from' &
          , Filename
        STOP
      ELSE
!
! End of file
!
        NULLIFY (Current_y%next)
      END IF
   END DO
!
! Data has now been read and stored in 2 linked lists
! start at the beginning of x linked list and
! y linked list and compare indices
! in order to perform inner product
!
   Current_x => Root_x
   Current_y => Root_y
   DO WHILE (ASSOCIATED(Current_x%next))
      DO WHILE (Associated(Current_y%next) &
       .AND. Current_y%index < Current_x%index)
!
! move through 2nd list
!
        Current_y => Current_y%next
      END DO
!
! At this point Current_y%index >= Current_x%index
! or 2nd list is exhausted
!
      IF (Current_y%index == Current_x%index) THEN
```

```
        Inner_prod = Inner_prod &
          + Current_x%value * Current_y%value
      END IF
      Current_x => Current_x%next
   END DO
!
! Print out inner product
!
   PRINT *,'Inner product of two sparse vectors is :' &
     , Inner_prod
!
! Print non-zero values of vector x and indices
!
   PRINT*, 'non-zero values of vector x and indices:'
   Current_x => Root_x
   DO WHILE (ASSOCIATED(Current_x%next))
      PRINT*,Current_x%value,Current_x%index
      Current_x => Current_x%next
   END DO
!
! Print non-zero values of vector y and indices
!
PRINT*, 'non-zero values of vector y and indices:'
   Current_y => Root_y
   DO WHILE (ASSOCIATED(Current_y%next))
      PRINT*,Current_y%value,Current_y%index
      Current_y => Current_y%next
   END DO
!
END PROGRAM ch2601
```

26.2 Solving a system of first-order ordinary differential equations using Runga–Kutta–Merson

Simulation and mathematical modelling of a wide range of physical processes often leads to a system of ordinary differential equations to be solved. Such equations also occur when approximate techniques are applied to more complex problems. We will restrict ourselves to a class of ordinary differential equations called initial value problems. These are systems for which all conditions are given at the same value of the independent variable. We will further restrict ourselves to first-order initial value problems of the form:

$$\frac{dy_1}{dt} = f_1(\underline{y}, t)$$
$$\frac{dy_2}{dt} = f_2(\underline{y}, t)$$
…
$$\frac{dy_n}{dt} = f_n(\underline{y}, t)$$

or

$$\dot{\underline{y}} = \underline{f}\ (\ \underline{y}\ , t\ ) \tag{1}$$

with initial conditions

$$\underline{y}(t0) = \underline{y}0$$

where

$$\underline{y} = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix} \qquad \underline{f} = \begin{pmatrix} f_1 \\ \vdots \\ f_n \end{pmatrix} \qquad \underline{y}_0 = \begin{pmatrix} y_1(t_0) \\ \vdots \\ y_n(t_0) \end{pmatrix}$$

If we have a system of ordinary differential equations of higher order then they can be reformulated to a system of order one. See the NAG library documentation for solving ordinary differential equations.

One well-known class of methods for solving initial value ordinary differential equations is Runge–Kutta. In this example we have coded the Runga–Kutta–Merson algorithm, which is a fourth-order method and solves (1) from a point $t = A$ to a point $t = B$.

It starts with a step length $h = (B - A) \,/\, 100$ and includes a local error control strategy such that the solution at $t+h$ is accepted if:

$$|error\ \ estimate| < \ \ user\ \ defined\ \ tolerance.$$

If this isn't satisfied the step length h is halved and the solution attempt is repeated until the above is satisfied or the step length is too small and the problem is left unsolved. If the error criterion is satisfied the algorithm progresses with a suitable step length solving the equations at intermediate points until the end point B is reached. For a full discussion of the algorithm and the error control mechanism used see *Numerical Methods in Practice* by Tim Hopkins and Chris Phillips:

```
MODULE Precisions
INTEGER,PARAMETER:: Long=SELECTED_REAL_KIND(15,307)
END MODULE Precisions
```

```
SUBROUTINE Runge_Kutta_Merson(Y,FUN,IFAIL,N,A,B,Tol)
!
! Runge-Kutta-Merson method for the solution
! of a system of N
! 1st order initial value ordinary
! differential equations.
! The routine tries to integrate from T=A to T=B with
! initial conditions in Y, subject to the
! condition that the
! Absolute Error Estimate <= Tol. The step length is
! adjusted automatically to meet this condition.
! If the routine is successful it returns with
! IFAIL = 0, T=B and
! the solution in Y.
!
USE Precisions
!
IMPLICIT NONE
! Define arguments
!
REAL (Long),INTENT(INOUT):: Y(:)
REAL(Long), INTENT(IN)::A,B,Tol
INTEGER,INTENT(IN)::N
INTEGER,INTENT(OUT)::IFAIL
!
INTERFACE
   SUBROUTINE FUN(T,Y,F,N)
   USE Precisions
   IMPLICIT NONE
   REAL(Long),INTENT(IN),DIMENSION(:)::Y
   REAL(Long),INTENT(OUT),DIMENSION(:)::F
   REAL(Long),INTENT(IN)::T
   INTEGER,INTENT(IN)::N
   END SUBROUTINE FUN
END INTERFACE
!
! Local variables
!
REAL(Long), DIMENSION(1:SIZE(Y)):: &
            S1,S2,S3,S4,S5,New_Y_1,New_Y_2,Error
REAL(Long)::T,H,H2,H3,H6,H8,Factor=1.E-2_Long
```

```
REAL(Long)::Smallest_step=1.E-6_Long,Max_Error
INTEGER::No_of_steps=0
!
   IFAIL=0
!
! Check input parameters
!
   IF(N <= 0 .OR. A == B .OR. Tol <= 0.0) THEN
      IFAIL = 1
      RETURN
   ENDIF
!
! Initialize T to be start of interval and
! H to be 1/100 of interval
   T=A
   H=(B-A)/100.0_Long
   DO                        ! Beginning of Repeat loop
      H2=H/2.0_Long
      H3=H/3.0_Long
      H6=H/6.0_Long
      H8=H/8.0_Long
!
! Calculate S1,S2,S3,S4,S5
!
! S1=F(T,Y)

      CALL FUN(T,Y,S1,N)

      New_Y_1=Y+H3*S1

! S2 = F(T+H/3,Y+H/3*S1)

      CALL FUN(T+H3,New_Y_1,S2,N)
      New_Y_1=Y+H6*S1+H6*S2

! S3=F(T+H/3,Y+H/6*S1+H/6*S2)

      CALL FUN(T+H3,New_Y_1,S3,N)

      New_Y_1=Y+H8*(S2+3.0_Long*S3)

! S4=F(T+H/2,Y+H/8*(S2+3*S3))
```

```
      CALL FUN(T+H2,New_Y_1,S4,N)
      New_Y_1=Y+H2*(S1-3.0_Long*S3+4.0_Long*S4)

! S5=F(T+H,Y+H/2*(S1-3*S3+4*S4))

      CALL FUN(T+H,New_Y_1,S5,N)
!
! Calculate values at T+H
!
      New_Y_1=Y+H6*(S1+4.0_Long*S4+S5)
      New_Y_2=Y+H2*(S1-3.0_Long*S3+4.0*S4)
!
! Calculate error estimate
!
      Error=ABS(0.2_Long*(New_Y_1-New_Y_2))
      Max_Error=MAXVAL(Error)
      IF(Max_Error > Tol) THEN
!
! Halve step length and try again
!
         IF(ABS(H2) < Smallest_step) THEN
            IFAIL = 2
            RETURN
         ENDIF
         H=H2
      ELSE
!
! Accepted approximation so overwrite Y with Y_new_1,
! and T with T+H
!
         Y=New_Y_1
         T=T+H
!
! Can next step be doubled?
!
         IF(Max_Error*Factor < Tol)THEN
            H=H*2.0_Long
         ENDIF
!
! Does next step go beyond interval end B,
! if so set H = B-T
```

```
!
         IF(T+H > B) THEN
            H=B-T
         ENDIF
         No_of_steps=No_of_steps+1
      ENDIF
      IF(T >= B) EXIT            ! End of repeat loop
   END DO
END SUBROUTINE Runge_Kutta_Merson
```

A main program to use this subroutine is of the form:

```
PROGRAM ch2602
USE Precisions
IMPLICIT NONE
REAL(Long),Dimension(:),Allocatable::Y
REAL(Long)::A,B,Tol
INTEGER::N,IFAIL,All_stat
INTERFACE
   SUBROUTINE Runge_Kutta_Merson(Y,FUN,IFAIL,N,A,B,Tol)
      USE Precisions
      IMPLICIT NONE
      REAL(Long),INTENT(INOUT) :: Y(:)
      REAL(Long),INTENT(IN)::A,B,Tol
      INTEGER,INTENT(IN)::N
      INTEGER,INTENT(OUT)::IFAIL
      INTERFACE
         SUBROUTINE FUN(T,Y,F,N)
            USE Precisions
            IMPLICIT NONE
            REAL(Long), INTENT(IN),DIMENSION(:)::Y
            REAL(Long), INTENT(OUT),DIMENSION(:)::F
            REAL(Long), INTENT(IN)::T
            INTEGER,INTENT(IN)::N
         END SUBROUTINE FUN
      END INTERFACE
   END SUBROUTINE Runge_Kutta_Merson
END INTERFACE
!
INTERFACE
   SUBROUTINE Fun1(T,Y,F,N)
   USE Precisions
   IMPLICIT NONE
```

```
   REAL(Long), INTENT(IN),DIMENSION(:)::Y
   REAL(Long), INTENT(OUT),DIMENSION(:)::F
   REAL(Long),INTENT(IN):: T
   INTEGER, INTENT(IN):: N
   END SUBROUTINE Fun1
END INTERFACE
!
   PRINT *,'Input no of equations'
   READ*,N
!
! Allocate space for Y - checking to see that it
! allocates properly
!
   ALLOCATE(Y(1:N),STAT=All_stat)
   IF(All_stat /= 0) THEN
      PRINT * , ' Not enough memory'
      PRINT * , ' array Y is not allocated'
      STOP
   ENDIF
   PRINT *,' Input start and end of interval over'
   PRINT *,' which equations to be solved'
   READ *,A,B
   PRINT *,"Input ic's"
   READ *,Y(1:N)
   PRINT *,'Input Tolerance'
   READ *,Tol
   PRINT *,'At T= ',A
   PRINT *,'Initial conditions are :',Y(1:N)
   CALL Runge_Kutta_Merson(Y,Fun1,IFAIL,N,A,B,Tol)
   IF(IFAIL /= 0) THEN
      PRINT *,'Integration stopped with IFAIL = ',IFAIL
   ELSE
      PRINT *,'at T= ',B
      PRINT*,'Solution is: ',Y(1:N)
   ENDIF
END PROGRAM ch2602
```

Consider trying to solve the following system of first-order ordinary differential equations:

$\dot{y}_1 = \tan y_3$

$$\dot{y}_2 = \frac{-0.032 \tan y_3}{y_2} - \frac{0.02\ y_2}{\cos y_3}$$

$$\dot{y}_3 = -\frac{0.032}{y_2^2}$$

over an interval $t = 0.0$ to $t = 8.0$ with initial conditions $y1 = 0 \quad y2 = 0.5 \quad y3 = \frac{\pi}{5}$

The user supplied subroutine is:

```
Subroutine Fun1(T,Y,F,N)
   USE Precisions
   IMPLICIT NONE
   REAL(Long),INTENT(IN),DIMENSION(:)::Y
   REAL(Long),INTENT(OUT),DIMENSION(:)::F
   REAL(Long),INTENT(IN)::T
   INTEGER,INTENT(IN)::N
!
   F(1)=TAN(Y(3))
   F(2)=-0.032_Long*F(1)/Y(2)-0.02_Long*Y(2)/COS(Y(3))
   F(3)=-0.032_Long/(Y(2)*Y(2))
END SUBROUTINE Fun1
```

26.2.1 Note: Alternative form of the ALLOCATE statement

In the main program Odes we have defined Y to be a deferred-shape array, allocating it space after the variable N is read in. In order to make sure that enough memory is available to allocate space to array Y the ALLOCATE statement is used as follows:

ALLOCATE(Y(1:N),STAT=All_stat)

If the allocation is successful variable All_stat returns zero; otherwise it is given a processor dependent positive value. We have included code to check for this and the program stops if All_stat is not zero.

26.2.2 Note: Automatic arrays

The subroutine Runge_Kutta_Merson needs a number of local rank 1 arrays S1, S2, S3, S4 and S5 for workspace, their shape and size being the same as the dummy argument Y. Fortran 95 supplies automatic arrays for this purpose and can be declared as

```
REAL(Long), DIMENSION (1:SIZE(Y)) :: S1, S2, S3, S4, S5
```

The size of automatic arrays can depend on the size of actual arrays: in our example they are the same shape and size as the dummy array Y, or some other dummy arguments. Automatic arrays are created when the procedure is called and destroyed when control passes back to the calling program unit. They may have different shapes and sizes with different calls to the procedure, and because of this automatic arrays cannot be saved or initialised.

A word of warning should be given at this point. If there isn't enough memory available when an automatic array needs to be created problems will occur. Unlike allocatable arrays there is no way of testing to see if an automatic array has been created successfully. The general feeling is that even though they are nice, automatic arrays should be used with care and perhaps shouldn't be used in production code!

26.2.3 Note: Dummy procedure arguments

In order to make the use of the subroutine Runge_Kutta_Merson as general as possible, one of its dummy arguments (FUN) is the name of a subroutine which the user supplies with the actual system of ordinary differential equations he or she wishes to solve. This means that the main program which calls Runge_Kutta_Merson passes as an actual argument the name of the subroutine containing the definition of the equations to be solved. In this example the subroutine is called Fun1. In order to do this in the main program Odes we have an interface block for the Runge_Kutta_Merson subroutine and within this interface block we have another interface block for the dummy routine FUN. We also have an interface block for the actual subroutine Fun1 in the main program.

26.2.4 Keyword and optional arguments

The examples of procedures so far have assumed that the dummy arguments and the corresponding arguments are in the same position, i.e., we are using positional arguments. Fortran 95 also provides the ability to supply the actual arguments to a procedure by keyword, and hence in any order.

To do this the name of the dummy argument is referred to as the keyword and is specified in the actual argument list in the form

```
dummy-argument = actual-argument
```

To illustrate this, let us consider a subroutine to solve ordinary differential equations. The full subroutine and explanation are given in Chapter 27:

```
SUBROUTINE Runge_Kutta_Merson(Y,FUN,IFAIL,N,A,B,TOL)
```

where A is the initial point, B is the end point at which the solution is required, TOL is the accuracy to which the solution is required and N is the number of equations. The rest of the dummy arguments are explained in Chapter 27.

The subroutine can be called as follows:

```
CALL Runge_Kutta_Merson( Y , Fun1 , IFAIL , A=0.0 ,&
    B=8.0 , Tol=1.0E-6 , N=3)
```

where the dummy arguments A, B, Tol and N are now being used as keywords. The use of keyword arguments makes the code easier to read and decreases the need to remember their precise position in the argument list.

Also with Fortran 95 comes the ability to specify that an argument is optional. This is very useful when designing procedures for use by a range of programmers. Inside a procedure defaults can be set for the optional arguments providing an easy-to-use interface, while at the same time allowing sophisticated users a more comprehensive one.

To declare a dummy argument to be optional the OPTIONAL attribute can be used. For example, the last dummy argument Tol for the subroutine Runge_Kutta_Merson could be declared to be optional (although internally in the subroutine the code would have to be changed to allow for this), e.g.,

```
SUBROUTINE Runge_Kutta_Merson(Y,FUN,IFAIL,N,A,B,Tol)
USE Precisions
   REAL(Long), INTENT(INOUT), OPTIONAL :: Tol
```

and because it is at the end of the dummy argument list, calling the subroutine with a positional argument list, Tol can be omitted, e.g.,

```
CALL Runge_Kutta_Merson(Y,Fun1,IFAIL,N,A,B)
```

The code of the subroutine will need to be changed to check to see if the argument Tol is supplied, the intrinsic function PRESENT being available for this purpose. Sample code is given below:

```
SUBROUTINE Runge_Kutta_Merson(Y,FUN, IFAIL, N,A,B,Tol)
USE Precisions
! code left out
REAL(Long),INTENT(IN),OPTIONAL::Tol
REAL(Long)::Internal_tol = 1.0D-3
   IF(PRESENT(Tol)) THEN
      Internal_tol=Tol
      PRINT*,'Tol = ', Internal_tol,' is supplied'
   ELSE
```

```
      PRINT*,"Tol isn't supplied, default tolerance = "
      PRINT *,Internal_tol,' is used'
   ENDIF
! code left out but all references to tol
! would have to be changed to internal_tol
END SUBROUTINE Runge_Kutta_Merson
```

A number of points need to be noted when using keyword and optional arguments:

- If all the actual arguments use keywords, they may appear in any order.
- When only some of the actual arguments use keywords, the first part of the list must be positional followed by keyword arguments in any order.
- When using a mixture of positional and keyword arguments, once a keyword argument is used all subsequent arguments must be specified by keyword.
- If an actual argument is omitted the corresponding optional dummy argument must not be redefined or referenced, except as an argument to the PRESENT intrinsic function.
- If an optional dummy argument is at the end of the argument list then it can just be omitted from the actual argument list.
- Keyword arguments are needed when an optional argument not at the end of an argument list is omitted, unless all the remaining arguments are omitted as well.
- Keyword and optional arguments require explicit procedure interfaces, i.e., the procedure must be internal, a module procedure or have an interface block available in the calling program unit.

A number of the intrinsic procedures we have used have optional arguments. Consult Appendix D for details.

26.3 Generic procedures

There has always been a degree of support in Fortran for the concept of a generic procedure. Simplistically, a procedure is generic if it can handle arguments of more than one data type. This concept is one that is probably taken for granted with the intrinsic procedures.

With Fortran 95 we can now define our own generic procedures. The example we will use is based on the earlier one of sorting. In the original example the program worked with real data. In the example below we have extended the program to handle both integer and real data.

What is not obvious from our use of the internal procedures is that there will be specific procedures to handle each data type, i.e., if a function can take integer, real and complex arguments then there will be one implementation of that function for each data type, i.e., three separate functions.

In the example below we add the ability to handle integer data. This means that where we had:

- read data
- sort data
- print data

and one subroutine to implement the above we now have **two** subroutines to do each of the above, one to handle integers and one to handle reals:

```
PROGRAM ch2603

use read_data_module
use sort_data_module
use print_data_module

IMPLICIT NONE
INTEGER :: How_Many
CHARACTER (LEN=20) :: File_Name
INTEGER , ALLOCATABLE , DIMENSION(:) :: integer_data
REAL    , ALLOCATABLE , DIMENSION(:) :: real_Data

   PRINT * , ' How many data items are there?'
   READ  * , How_Many
   PRINT * , ' What is the file name?'
   READ '(A)',File_Name
   ALLOCATE(integer_data(How_Many))
   CALL Read_Data(File_Name,integer_data,How_Many)
   CALL Sort_Data(integer_data,How_Many)
   CALL Print_Data(integer_data,How_Many)
   PRINT *, ' Phase 1 ends.'
   PRINT *, ' data written to file name ISORTED.DAT'
   DEALLOCATE(integer_data)

   PRINT * , ' How many data items are there?'
   READ  * , How_Many
   PRINT * , ' What is the file name?'
   READ '(A)',File_Name
```

```
   ALLOCATE(real_data(How_Many))
   CALL Read_Data(File_Name,real_data,How_Many)
   CALL Sort_Data(real_data,How_Many)
   CALL Print_Data(real_data,How_Many)
   PRINT *, ' Program ends.'
   PRINT *, ' data written to file name RSORTED.DAT'
END PROGRAM ch2603

module read_data_module

interface read_data

   module procedure read_integer
   module procedure read_real

end interface read_data

contains

SUBROUTINE read_real(File_Name,Raw_Data,How_Many)
IMPLICIT NONE
CHARACTER (LEN=*) , INTENT(IN) :: File_Name
INTEGER , INTENT(IN) :: How_Many
REAL , INTENT(OUT) , &
   DIMENSION(:) :: Raw_Data
INTEGER :: I
   OPEN(FILE=File_Name,UNIT=1)
   DO I=1,How_Many
      READ (UNIT=1,FMT=*) Raw_Data(I)
   ENDDO
END SUBROUTINE read_real

SUBROUTINE read_integer(File_Name,Raw_Data,How_Many)
IMPLICIT NONE
CHARACTER (LEN=*) , INTENT(IN):: File_Name
INTEGER , INTENT(IN) :: How_Many
INTEGER , INTENT(OUT) , &
   DIMENSION(:) :: Raw_Data
INTEGER :: I
   OPEN(FILE=File_Name,UNIT=1)
   DO I=1,How_Many
      READ (UNIT=1,FMT=*) Raw_Data(I)
```

```
   ENDDO
END SUBROUTINE read_integer

end module read_data_module

module sort_data_module

interface sort_data

   module procedure sort_integer
   module procedure sort_real

end interface sort_data

contains

SUBROUTINE sort_real(Raw_Data,How_Many)
IMPLICIT NONE
INTEGER , INTENT(IN) :: How_Many
REAL , INTENT(INOUT)  , &
   DIMENSION(:) :: Raw_Data
   CALL QuickSort(1,How_Many)

CONTAINS

RECURSIVE SUBROUTINE QuickSort(L,R)
IMPLICIT NONE
INTEGER , INTENT(IN) :: L,R
INTEGER :: I,J
REAL :: V,T

   i=l
   j=r
   v=raw_data( int((l+r)/2) )
   do
      do while (raw_data(i) < v )
           i=i+1
      enddo
      do while (v < raw_data(j) )
           j=j-1
      enddo
      if (i<=j) then
```

```
        t=raw_data(i)
        raw_data(i)=raw_data(j)
        raw_data(j)=t
        i=i+1
        j=j-1
      endif
      if (i>j) exit
   enddo

   if (l<j) then
      call quicksort(l,j)
   endif

   if (i<r) then
      call quicksort(i,r)
   endif

END SUBROUTINE QuickSort

END SUBROUTINE sort_real

SUBROUTINE sort_integer(Raw_Data,How_Many)
IMPLICIT NONE
INTEGER , INTENT(IN) :: How_Many
INTEGER , INTENT(INOUT)   , &
   DIMENSION(:) :: Raw_Data
   CALL QuickSort(1,How_Many)

CONTAINS

RECURSIVE SUBROUTINE QuickSort(L,R)
IMPLICIT NONE
INTEGER , INTENT(IN) :: L,R
INTEGER :: I,J
INTEGER :: V,T

   i=l
   j=r
   v=raw_data( int((l+r)/2) )
   do
      do while (raw_data(i) < v )
           i=i+1
```

```
     enddo
     do while (v < raw_data(j) )
          j=j-1
     enddo
     if (i<=j) then
       t=raw_data(i)
       raw_data(i)=raw_data(j)
       raw_data(j)=t
       i=i+1
       j=j-1
     endif
     if (i>j) exit
   enddo

   if (l<j) then
     call quicksort(l,j)
   endif

   if (i<r) then
     call quicksort(i,r)
   endif

END SUBROUTINE QuickSort

END SUBROUTINE sort_integer

end module sort_data_module

module print_data_module

interface print_data

   module procedure print_integer
   module procedure print_real

end interface print_data

contains

SUBROUTINE print_real(Raw_Data,How_Many)
IMPLICIT NONE
INTEGER , INTENT(IN) :: How_Many
```

```
REAL , INTENT(IN) , &
   DIMENSION(:) :: Raw_Data
INTEGER :: I
  OPEN(FILE='RSORTED.DAT',UNIT=2)
  DO I=1,How_Many
    WRITE(UNIT=2,FMT=*) Raw_Data(I)
  END DO
  CLOSE(2)
END SUBROUTINE print_real

SUBROUTINE print_integer(Raw_Data,How_Many)
IMPLICIT NONE
INTEGER , INTENT(IN) :: How_Many
INTEGER , INTENT(IN) , &
   DIMENSION(:) :: Raw_Data
INTEGER :: I
  OPEN(FILE='ISORTED.DAT',UNIT=2)
  DO I=1,How_Many
    WRITE(UNIT=2,FMT=*) Raw_Data(I)
  END DO
  CLOSE(2)
END SUBROUTINE print_integer

end module print_data_module
```

The key code is given below for each module:

```
interface read_data

  module procedure read_integer
  module procedure read_real

end interface read_data

interface sort_data

  module procedure sort_integer
  module procedure sort_real

end interface sort_data

interface print_data
```

```
   module procedure print_integer
   module procedure print_real

end interface print_data
```

The interface block name is used in the calling routine and the appropriate module procedure will be called, based on a signature match of the actual and dummy parameters.

26.4 A function that returns a variable length array

The following program illustrates the use of a function that returns a variable length array. This is in Fortran 90 style. The program also shows a second way of generic programming using explicit interfaces. In this case you again use the interface name in the calling routine, and the appropriate routine is called on the basis of a parameter signature match:

```
PROGRAM ch2604
IMPLICIT NONE

INTERFACE
   FUNCTION Running_Average(R,How_Many)
      IMPLICIT NONE
      INTEGER , INTENT(IN) :: How_Many
      REAL , DIMENSION (:) , INTENT(IN) :: R
      REAL , DIMENSION(how_many) :: Running_Average
   END FUNCTION Running_Average
END INTERFACE

INTERFACE Read_Data

   SUBROUTINE RR(File_Name,Raw_Data,How_Many)
      IMPLICIT NONE
      CHARACTER (LEN=*) , INTENT(IN) :: File_Name
      INTEGER , INTENT(IN) :: How_Many
      REAL , INTENT(OUT) , &
      DIMENSION(:) :: Raw_Data
   END SUBROUTINE RR

   SUBROUTINE RI(File_Name,Raw_Data,How_Many)
      IMPLICIT NONE
      CHARACTER (LEN=*) , INTENT(IN) :: File_Name
      INTEGER , INTENT(IN) :: How_Many
```

```
      INTEGER , INTENT(OUT) , &
      DIMENSION(:) :: Raw_Data
   END SUBROUTINE RI

END INTERFACE

INTEGER :: How_Many
CHARACTER (LEN=20) :: File_Name
REAL , ALLOCATABLE , DIMENSION(:)   :: Raw_Data
REAL , ALLOCATABLE , DIMENSION(:)   :: RA
INTEGER :: I
   PRINT * , ' How many data items are there?'
   READ  * , How_Many
   PRINT * , ' What is the file name?'
   READ '(A)',File_Name
   ALLOCATE(Raw_Data(how_many))
   ALLOCATE(RA(how_many))
   CALL Read_Data(File_Name,Raw_Data,How_Many)
   RA=Running_Average(Raw_Data,How_Many)
   DO I=1,How_Many
      PRINT *,Raw_Data(I),'    ' ,RA(I)
   END DO
END PROGRAM ch2604

FUNCTION Running_Average(R,How_Many)
INTEGER , INTENT(IN) :: How_Many
REAL , INTENT(IN) , DIMENSION(:) :: R
REAL , DIMENSION(how_many) :: Running_Average
INTEGER :: I
REAL :: Sum=0.0
   DO I=1,How_Many
      Sum = Sum + R(I)
      Running_Average(I)=Sum/I
   END DO
END FUNCTION Running_Average

SUBROUTINE RR(File_Name,Raw_Data,How_Many)
IMPLICIT NONE
CHARACTER (LEN=*) , INTENT(IN) :: File_Name
INTEGER , INTENT(IN) :: How_Many
REAL , INTENT(OUT) , &
   DIMENSION(:) :: Raw_Data
```

```
INTEGER :: I
  OPEN(FILE=File_Name,UNIT=1)
  DO I=1,How_Many
    READ (UNIT=1,FMT=*) Raw_Data(I)
  ENDDO
END SUBROUTINE RR

SUBROUTINE RI(File_Name,Raw_Data,How_Many)
IMPLICIT NONE
CHARACTER (LEN=*) , INTENT(IN):: File_Name
INTEGER , INTENT(IN) :: How_Many
INTEGER , INTENT(OUT) , &
   DIMENSION(:) :: Raw_Data
INTEGER :: I
  OPEN(FILE=File_Name,UNIT=1)
  DO I=1,How_Many
    READ (UNIT=1,FMT=*) Raw_Data(I)
  ENDDO
END SUBROUTINE RI
```

The preferred way of doing this is shown in Chapter 28, but it only works with compilers that support ISO TR 15581.

26.5 Operator and assignment overloading

It is sometimes convenient to extend the meaning of an operator and the assignment symbol beyond that provided by the language. This can be done in Fortran 95 using module procedures. The example below is based on moving around a three-dimensional space:

```
MODULE T_Position
IMPLICIT NONE
TYPE Position
   INTEGER :: X
   INTEGER :: Y
   INTEGER :: Z
END TYPE Position

INTERFACE OPERATOR (+)
   MODULE PROCEDURE New_Position
END INTERFACE

CONTAINS
```

```
FUNCTION New_Position(A,B)
TYPE (Position) ,INTENT(IN) :: A,B
TYPE (Position) :: New_Position
   New_Position % X = A % X + B % X
   New_Position % Y = A % Y + B % Y
   New_Position % Z = A % Z + B % Z
END FUNCTION New_Position

END MODULE T_Position

PROGRAM ch2605
USE T_Position
IMPLICIT NONE
TYPE (Position) :: A,B,C
   A%X=10
   A%Y=10
   A%Z=10
   B%X=20
   B%Y=20
   B%Z=20
   C=A+B
   PRINT *,A
   PRINT *,B
   PRINT *,C
END PROGRAM ch2605
```

We have extended the meaning of the addition operator so that we can write simple expressions in Fortran based on it and have our new position calculated using a user supplied function that actually implements the calculation of the new position.

26.6 A subroutine to extract the diagonal elements of a matrix

A common task mathematically is to extract the diagonal elements of a matrix. For example if

$$A = \begin{pmatrix} 21 & 6 & 7 \\ 9 & 3 & 2 \\ 4 & 1 & 8 \end{pmatrix}$$

the diagonal elements are (21, 3, 8).

This can be thought of as extracting an array section, but the intrinsic function PACK is needed. In its simplest form PACK (Array,Vector) packs an array, Array, into a rank 1 array, Vector, according to Array's array element order.

Below is a complete program to demonstrate this:

```
PROGRAM ch2606
IMPLICIT NONE
INTEGER::I, N
REAL, ALLOCATABLE, DIMENSION(:,:) :: A
REAL, ALLOCATABLE, DIMENSION(:):: Adiag
LOGICAL:: OK
CHARACTER(LEN=20)::Filename

INTERFACE
  SUBROUTINE Matrix_Diagonal (A, Diag, N, OK)
    IMPLICIT NONE
    REAL, INTENT(IN), DIMENSION(:,:) ::A
    REAL, INTENT(OUT), DIMENSION(:) :: Diag
    INTEGER, INTENT(IN) ::N
    LOGICAL, INTENT(OUT):: OK
  END SUBROUTINE Matrix_Diagonal
END INTERFACE

  PRINT*,'input name of data file'
  READ '(A)',Filename
  OPEN(UNIT=1,FILE=Filename)
  READ(1,*) N
  ALLOCATE(A(1:N,1:N), Adiag(1:N))
  DO I=1,N
    READ(1,*)A(I,1:N)
  END DO
  CALL Matrix_Diagonal(A,Adiag,N, OK)
  IF(OK) THEN
    PRINT*,' Diagonal elements of A are:'
    PRINT *,Adiag
  ELSE
    PRINT*,'Matrix A is not square'
  END IF
END PROGRAM ch2606

SUBROUTINE Matrix_Diagonal (A, Diag, N, OK)
IMPLICIT NONE
```

```
REAL, INTENT(IN), DIMENSION(:,:) ::A
REAL, INTENT(OUT), DIMENSION(:) :: Diag
INTEGER, INTENT(IN) ::N
LOGICAL, INTENT(OUT):: OK
REAL, DIMENSION (1:SIZE(A,1)*SIZE(A,1)) :: Temp
!
! Subroutine to extract the diagonal elements of
! an N * N matrix A
!
  IF(SIZE(A,1) == N .AND. SIZE(A,2) == N) THEN
!   Matrix is square
    OK=.TRUE.
    Temp = PACK(A,.TRUE.)
    Diag=Temp(1:N*N:N+1)
  ELSE
!   Matrix isn't square
    OK=.FALSE.
  END IF
END SUBROUTINE Matrix_Diagonal
```

26.7 Perfectly balanced tree

Let us now look at a more complex example that builds a perfectly balanced tree and prints it out. A loose definition of a perfectly balanced tree is one that has minimum depth for *n* nodes. More accurately a tree is perfectly balanced if for each node the number of nodes in its left and right subtrees differ by at most 1:

```
MODULE Node_Type_Def
IMPLICIT NONE
  TYPE Tree_Node
  INTEGER :: Number
  TYPE (Tree_Node) , POINTER :: Left,Right
  END TYPE Tree_Node
END MODULE Node_Type_Def

PROGRAM ch2607
! Construction of a perfectly balanced tree
USE Node_Type_Def
IMPLICIT NONE
TYPE (Tree_Node) , POINTER :: Root
INTEGER :: N_of_Items

INTERFACE
```

```
   RECURSIVE FUNCTION Tree(N) RESULT(Answer)
     USE Node_Type_Def
     IMPLICIT NONE
     INTEGER , INTENT(IN) :: N
     TYPE (Tree_Node) , POINTER :: Answer
   END FUNCTION Tree

   SUBROUTINE Print_Tree(Trees,H)
     USE Node_Type_Def
     IMPLICIT NONE
     TYPE (Tree_Node) , POINTER :: Trees
     INTEGER :: H
   END SUBROUTINE Print_Tree

END INTERFACE

   PRINT *,' Enter number of items'
   READ *,N_Of_Items
   Root=>Tree(N_Of_Items)
   CALL Print_Tree(Root,0)

END PROGRAM ch2607

RECURSIVE FUNCTION Tree(N) RESULT (Answer)
USE Node_Type_Def
IMPLICIT NONE
INTEGER , INTENT(IN) :: N
TYPE (Tree_Node) , POINTER :: Answer
TYPE (Tree_Node) , POINTER :: New_Node

INTEGER :: L,R,X
   IF (N == 0) THEN
     print *,' terminate tree'
     NULLIFY(Answer)
   ELSE
     L=N/2
     R=N-L-1
     PRINT *,L,R,N
     PRINT *,' Next item'
     READ *,X
     ALLOCATE(New_Node)
```

```
      New_Node%Number=X
      print *, ' left branch'
      New_Node%Left => Tree(L)
      print *, ' right branch'
      New_Node%Right => Tree(R)
      Answer => New_Node
   ENDIF
   PRINT *, ' Function tree ends'
END FUNCTION Tree

RECURSIVE SUBROUTINE Print_Tree(T,H)
USE Node_Type_Def
IMPLICIT NONE
TYPE (Tree_Node) , POINTER :: T
INTEGER :: I
INTEGER :: H
   IF (ASSOCIATED(T)) THEN
      CALL Print_Tree(T%Left,H+1)
      DO I=1,H
         WRITE(UNIT=*,FMT=10,ADVANCE='NO')
         10 FORMAT('    ')
      ENDDO
      PRINT *,T%Number
      CALL Print_Tree(T%Right,H+1)
   ENDIF
END SUBROUTINE Print_Tree
```

There are a number of very important concepts contained in this example and they include:

- The use of a module to define a type. For user defined data types we must create a module to define the data type if we want it to be available in more than one program unit.
- The use of a function that returns a pointer as a result.
- As the function returns a pointer we must determine the allocation status before the function terminates. This means that in the above case we use the NULLIFY(Result) statement. The other option is to TARGET the pointer.
- The use of ASSOCIATED to determine if the node of the tree is terminated or points to another node.

Type the program in and compile, link and run it. Note that the tree only has the minimal depth necessary to store all of the items. Experiment with the number of items and watch the tree change its depth to match the number of items.

26.8 Pure function example

We recommended in Chapter 14 that you should ensure that your functions do not have side effects, for safety reasons. With the ability to run your code on parallel systems we have the additional problem in that the code may not actually work! We would also like to be able to take advantage of automatic parallelisation if possible. In the following example we show how to do this using the PURE function prefix:

```
PROGRAM ch2608
IMPLICIT NONE
INTEGER :: I,J,Result
INTEGER :: GCD
   PRINT *,' Type in two integers'
   READ *,I,J
   Result=GCD(I,J)
   PRINT *,' GCD is ',Result
END PROGRAM ch2608

PURE INTEGER FUNCTION GCD(A,B)
IMPLICIT NONE
INTEGER , INTENT(IN) :: A,B
INTEGER :: Temp
   IF (A < B) THEN
      Temp=A
   ELSE
      Temp=B
   ENDIF
   DO WHILE ((MOD(A,Temp) /= 0) .OR. (MOD(B,Temp) /=0))
      Temp=Temp-1
   END DO
   GCD=Temp
END FUNCTION GCD
```

Procedures can also be made pure.

26.8.1 Pure constraints

The following are some of the constraints on pure procedures:

- A dummy argument must be INTENT(IN) for a pure function.

- A dummy argument must have an INTENT attribute in a pure subroutine.
- Local variables may not have the save attribute.
- No I/O must be done in the procedure.
- Any functions and procedures referenced must be pure.
- You cannot have a stop statement with a pure procedure.

The above information should be enough to enable you to write simple pure functions and procedures.

26.9 Elemental function example

The intrinsic trigonometric functions are elemental in that they can take an argument that is scalar or array valued, and of any of the supported numeric kind types. With Fortran 95 we can make our own user defined functions elemental. Consider the following example, which is an extension of the earlier example that calculated e**x:

```
PROGRAM ch2609
IMPLICIT NONE
!
! Elemental function example
!
INTEGER :: I
REAL :: X
REAL , DIMENSION(10) :: Y

INTERFACE
   ELEMENTAL REAL FUNCTION ETOX(X)
   IMPLICIT NONE
   REAL , INTENT(IN) :: X
   END FUNCTION ETOX
END INTERFACE

   X=1.0
   DO I=1,10
      Y(I)=I
   END DO
   PRINT *,Y
   X=ETOX(X)
   PRINT *,X
   Y=ETOX(Y)
   PRINT *,Y
```

```
END PROGRAM ch2609

ELEMENTAL REAL FUNCTION ETOX(X)
IMPLICIT NONE
REAL , INTENT(IN) :: X
REAL :: TERM
INTEGER :: NTERM
REAL , PARAMETER :: TOL =1.0E-6
   ETOX=1.0
   TERM=1.0
   NTERM=0
   DO
      NTERM=NTERM+1
      TERM=(X/NTERM)*TERM
      ETOX=ETOX+TERM
      IF (TERM<=TOL) EXIT
   END DO
END FUNCTION ETOX
```

Note the following:

- We have added an interface block for the etox function.
- We have added the ELEMENTAL prefix to the function header.
- The dummy argument is scalar and INTENT(IN).
- The function result is scalar.

In this example we call the function with a scalar argument and a rank 1 array. Run the program to see what happens.

You can have the PURE prefix but it is redundant as ELEMENTAL implies PURE.

26.9.1 Elemental constraints

Some of the restrictions include:

- An elemental procedure must not be recursive.
- A dummy argument must not be a pointer.
- The result of an elemental function must not be a pointer.
- Elemental procedures must have explicit interfaces in all program units that reference them.

In a parallel environment this means that the array calculations could be carried out simultaneously on two or more processors.

26.10 Elemental subroutine example

It is also possible to make subroutines elemental. Consider the following example:

```
PROGRAM ch2610
IMPLICIT NONE

INTERFACE
   ELEMENTAL SUBROUTINE SWAP(X,Y)
   INTEGER , INTENT(INOUT) :: X,Y
   END SUBROUTINE SWAP
END INTERFACE

INTEGER , DIMENSION(10) :: A,B
INTEGER :: I
   DO I=1,10
      A(I)=I
      B(I)=I*I
   END DO
      PRINT *,A
      PRINT *,B
      CALL SWAP(A,B)
      PRINT *,A
      PRINT *,B
END PROGRAM ch2610

ELEMENTAL SUBROUTINE SWAP(X,Y)
INTEGER , INTENT(INOUT) :: X,Y
INTEGER :: TEMP
   TEMP=X
   X=Y
   Y=TEMP
END SUBROUTINE SWAP
```

Note the following:

- We have an interface block for the elemental subroutine.
- The subroutine dummy arguments are scalar with an INTENT attribute, in this case INTENT(INOUT) as we are swapping them over.

In a parallel environment the swapping of array elements may be done simultaneously on two or more processors.

26.11 Date class

The following is a complete manual rewrite of Skip Noble and Alan Millers date module. The original worked with the built-in Fortran intrinsic data types. It has been rewritten to work with a user defined or derived date data type.

The first key code segment is

```
TYPE, PUBLIC :: date
   PRIVATE
   INTEGER :: day
   INTEGER :: month
   INTEGER :: year
END TYPE date
```

where the date data type is public but its components are private. This means that access to the components must be done via subroutines and functions within the date_module module.

The next key code segment is

```
PUBLIC :: calendar_to_julian,&
   date_, &
   date_stamp, &
   date_to_day_in_year, &
   date_to_weekday_number, &
   get_day, &
   get_month, &
   get_year, &
   julian_to_date, &
   julian_to_date_and_week_and_day, &
   ndays, &
   year_and_day_to_date
```

where we explicitly make the listed subroutines and functions public, as the code segment from the top of the module,

```
! ..
! .. Default Accessibility ..
   PRIVATE
```

defines everything to be private.

We have to provide a user defined constructor when the components of the derived type are private. This is given below:

```
   FUNCTION date_(dd,mm,yyyy) RESULT (x)
!  .. Implicit None Statement ..
      IMPLICIT NONE
!  ..
!  .. Function Return Value ..
      TYPE (date) :: x
!  ..
!  .. Scalar Arguments ..
      INTEGER, INTENT (IN) :: dd, mm, yyyy
!  ..
      x = date(dd,mm,yyyy)
   END FUNCTION date_
```

This in turn calls the built-in constructor date.

We also provide three additional procedures to access the components of the date class:

```
get_day
get_month
get_year
```

This is common programming practice in object oriented and object based programming.

The program has also been through the Nag tool suite and this has helped to systematically lay out the code.

```
MODULE date_module
!   Collected and put together january 1972,
!   h. d. knoble.
!   Original references are cited in each routine.
!   Code converted using to_f90 by alan miller
!   Date: 1999-12-22  time: 10:23:47
!   Compatible with imagine1 f compiler: 2002-07-19
!   At this time the functions and
!   subroutines were as described below
!   FUNCTION iday(yyyy, mm, dd) RESULT(ival)
!   FUNCTION izlr(yyyy, mm, dd) RESULT(ival)
!   SUBROUTINE calend(yyyy, ddd, mm, dd)
!   SUBROUTINE cdate(jd, yyyy, mm, dd)
```

```
!   SUBROUTINE daysub(jd, yyyy, mm, dd, wd, ddd)
!   FUNCTION jd(yyyy, mm, dd) RESULT(ival)
!   FUNCTION ndays(mm1, dd1, yyyy1,
!       mm2, dd2, yyyy2) RESULT(ival)
!   SUBROUTINE date_stamp( string, want_day, short )
!   Code converted by ian chivers and jane sleightholme
!   November 2004 - May 2005
!   The changes are to go from
!   working with integer variables
!   for year, day and month to
!   user defined date variables.
! .. Implicit None Statement ..
  IMPLICIT NONE
! ..
! .. Default Accessibility ..
  PRIVATE
! ..
! .. Derived Type Declarations ..
  TYPE, PUBLIC :: date
    PRIVATE
    INTEGER :: day
    INTEGER :: month
    INTEGER :: year
  END TYPE date
! ..
! .. Public Statements ..
  PUBLIC :: calendar_to_julian,&
    date_, &
    date_stamp, &
    date_to_day_in_year, &
    date_to_weekday_number, &
    get_day, &
    get_month, &
    get_year, &
    julian_to_date, &
    julian_to_date_and_week_and_day, &
    ndays, &
    year_and_day_to_date
! ..
!   The above are the contained
!   functions and subroutines
!   in this module.
```

```
!  Here is a short description of each one
!     date_to_day_in_year      - function
!       returns the day in the year
!       original arguments of day,month,year
!       now date
!       dayinyear
!     date_to_weekday_number   - function
!       returns the week day number
!       original argument d,m,y
!       now date
!       weekdaynum
!     year_and_day_to_date     - subroutine
!       returns the day and month from
!       year and day in year
!     julian_to_date            - subroutine
!       returns a year_and_day_to_datear date from
!       a julian date
!     ndays                        - function
!       returns the number of days between
!       two dates
!     julian_to_date_and_week_and_day    - subroutine
!       given a julian day this routine
!       calculates year, month day and
!       week day number and day number
!     calendar_to_julian       - function
!       returns julian date from
!       year_and_day_to_datear date
CONTAINS

! arithmetic functions "izlr" and "iday"
! are taken from remark on
! algorithm 398, by j. douglas robertson,
! cacm 15(10):918.

   FUNCTION date_to_day_in_year(x)
! Convert from date to day in year
! .. Implicit None Statement ..
     IMPLICIT NONE
! ..
! .. Function Return Value ..
     INTEGER :: date_to_day_in_year
! ..
```

```
! .. Structure Arguments ..
     TYPE (date), INTENT (IN) :: x
! ..
! .. Intrinsic Functions ..
     INTRINSIC modulo
! ..
     date_to_day_in_year = 3055*(x%month+2)/100 &
       - (x%month+10)/13*2 - 91 + &
       (1-(modulo(x%year,4)+3)/4 &
       + (modulo(x%year,100)+99)/100 &
       - (modulo(x%year, &
       400)+399)/400)*(x%month+10)/13 + x%day

   END FUNCTION date_to_day_in_year

   FUNCTION date_to_weekday_number(x)
! .. Implicit None Statement ..
     IMPLICIT NONE
! ..
! .. Function Return Value ..
     INTEGER :: date_to_weekday_number
! ..
! .. Structure Arguments ..
     TYPE (date), INTENT (IN) :: x
! ..
! .. Intrinsic Functions ..
     INTRINSIC modulo
! ..
     date_to_weekday_number = &
       modulo((13*(x%month+10 &
       -(x%month+10)/13*12)-1)/5+x &
       %day+77+5*(x%year+(x%month-14)/12 &
       -(x%year+(x%month-14)/12)/100*100)/4 &
       +(x%year+(x%month-14)/12)/400 &
       -(x%year+(x%month-14)/12)/100*2,7)

   END FUNCTION date_to_weekday_number

   FUNCTION year_and_day_to_date(year,day) RESULT (x)
! .. Implicit None Statement ..
     IMPLICIT NONE
! ..
```

```
! .. Function Return Value ..
     TYPE (date) :: x
! ..
! .. Scalar Arguments ..
     INTEGER, INTENT (IN) :: day, year
! ..
! .. Local Scalars ..
     INTEGER :: t
! ..
! .. Intrinsic Functions ..
     INTRINSIC modulo
! ..
     x%year = year
     t = 0
     IF (modulo(year,4)==0) THEN
       t = 1
     END IF

!------the following statement is
! necessary IF year is < 1900 or > 2100.

     IF (modulo(year,400)/=0 &
       .AND. modulo(year,100)==0) THEN
       t = 0
     END IF

     x%day = day

     IF (day>59+t) THEN
       x%day = x%day + 2 - t
     END IF

     x%month = ((x%day+91)*100)/3055
     x%day = (x%day+91) - (x%month*3055)/100
     x%month = x%month - 2

     IF (x%month>=1 .AND. x%month<=12) THEN
       RETURN
     END IF

! x%month will be correct
! iff day is correct for year.
```

```
      WRITE (unit=*,fmt='(a,i11,a)') &
      '$$year_and_day_to_date: day of the year input =',
&
      day, ' is out of range.'

   END FUNCTION year_and_day_to_date



   FUNCTION julian_to_date(julian) RESULT (x)
! Given a julian day number the date is returned.
! julian is the julian date from an epocch
! in the very distant past.  see cacm 1968 11(10):657,
! letter to the editor by fliegel and van flandern.
! .. Implicit None Statement ..
      IMPLICIT NONE
! ..
! .. Scalar Arguments ..
      INTEGER, INTENT (IN) :: julian
! ..
! .. Local Scalars ..
      INTEGER :: l, n
! ..
! .. Function Return Value ..
      TYPE (date) :: x
! ..
      l = julian + 68569
      n = 4*l/146097
      l = l - (146097*n+3)/4
      x%year = 4000*(l+1)/1461001
      l = l - 1461*x%year/4 + 31
      x%month = 80*l/2447
      x%day = l - 2447*x%month/80
      l = x%month/11
      x%month = x%month + 2 - 12*l
      x%year = 100*(n-49) + x%year + l

   END FUNCTION julian_to_date


   SUBROUTINE &
```

```
  julian_to_date_and_week_and_day(jd,x,wd,ddd)
! given jd, a julian day # (see asf jd),
! this routine calculates dd,
! the day number of the month;
! mm, the month number; yyyy the year;
! wd the weekday number, and
! ddd the day number of the year.
! example:
! CALL julian_to_date_and_week_and_day
! (2440588, yyyy, mm, dd, wd, ddd)
! yields 1970 1 1 4 1.
! .. Implicit None Statement ..
    IMPLICIT NONE
! ..
! .. Scalar Arguments ..
    INTEGER, INTENT (OUT) :: ddd, wd
    INTEGER, INTENT (IN) :: jd
! ..
! .. Structure Arguments ..
    TYPE (date), INTENT (OUT) :: x
! ..
    x = julian_to_date(jd)
    wd = date_to_weekday_number(x)
    ddd = date_to_day_in_year(x)

  END SUBROUTINE julian_to_date_and_week_and_day


  FUNCTION calendar_to_julian(x) RESULT (ival)
! .. Implicit None Statement ..
    IMPLICIT NONE
! ..
! .. Function Return Value ..
    INTEGER :: ival
! ..
! .. Structure Arguments ..
    TYPE (date), INTENT (IN) :: x
! ..
! date routine calendar_to_julian converts date to
! julian date.  see cacm 1968 11(10):657,
! letter to the
! editor by henry f. fliegel and
```

```
! thomas c. van flandern.
! example calendar_to_julian(1970, 1, 1) = 2440588
     ival = x%day - 32075 &
       + 1461*(x%year+4800+(x%month-14)/12)/4 + &
       367*(x%month-2-((x%month-14)/12)*12)/12 &
       - 3*((x%year+4900+(x%month-14)/ &
       12)/100)/4

   END FUNCTION calendar_to_julian


   FUNCTION ndays(date1,date2)
! .. Implicit None Statement ..
     IMPLICIT NONE
! ..
! .. Function Return Value ..
     INTEGER :: ndays
! ..
! .. Structure Arguments ..
     TYPE (date), INTENT (IN) :: date1, date2
! ..
! dates; that is  mm1/dd1/yyyy1 minus
! mm2/dd2/yyyy2,
! where datei and datej have elements mm, dd, yyyy.
! ndays will be positive iff
! date1 is more recent than date2.
     ndays = calendar_to_julian(date1) &
       - calendar_to_julian(date2)

   END FUNCTION ndays

   SUBROUTINE date_stamp(string,want_day,short)
! Returns the current date as a character string
! e.g.
! want_day      short       string
! .TRUE.       .TRUE.       Thursday, 23 Dec 1999
! .TRUE.       .FALSE.      Thursday, 23 December 1999

!  <- defaul/
! .FALSE.      .TRUE.       23 Dec 1999
! .FALSE.      .FALSE.      23 December 1999
! .. Implicit None Statement ..
```

```
      IMPLICIT NONE
!  ..
!  .. Scalar Arguments ..
      LOGICAL, OPTIONAL, INTENT (IN) :: short, want_day
      CHARACTER (*), INTENT (OUT) :: string
!  ..
!  .. Local Scalars ..
      INTEGER :: pos
      LOGICAL :: sh, want_d
!  ..
!  .. Local Arrays ..
      INTEGER :: val(8)
      CHARACTER (9) :: day(0:6) = (/ 'Sunday    ' &
                                   , 'Monday    ' &
                                   , 'Tuesday   ' &
                                   ,  'Wednesday' &
                                   , 'Thursday  ' &
                                   , 'Friday    ' &
                                   , 'Saturday  '/)
      CHARACTER (9) :: month(1:12) = &
          (/ 'January   ' &
           , 'February  ' &
             , 'March     ' &
             , 'April     ' &
             , 'May       ' &
             , 'June      ' &
             , 'July      ' &
             , 'August    ' &
             , 'September' &
             , 'October   ' &
             , 'November  ' &
             , 'December  '/)
!  ..
!  .. Intrinsic Functions ..
      INTRINSIC date_and_time, len_trim, present, trim
!  ..
!  .. Local Structures ..
      TYPE (date) :: x
!  ..
      want_d = .TRUE.
      IF (present(want_day)) want_d = want_day
      sh = .FALSE.
```

```
    IF (present(short)) sh = short

    CALL date_and_time(values=val)

    x = date_(val(3),val(2),val(1))

    IF (want_d) THEN
      pos = date_to_weekday_number(x)
      string = trim(day(pos)) // ','
      pos = len_trim(string) + 2
    ELSE
      pos = 1
      string = ' '
    END IF

    WRITE (string(pos:pos+1),'(i2)') val(3)
    IF (sh) THEN
      string(pos+3:pos+5) = month(val(2)) (1:3)
      pos = pos + 7
    ELSE
      string(pos+3:) = month(val(2))
      pos = len_trim(string) + 2
    END IF

    WRITE (string(pos:pos+3),'(i4)') val(1)

    RETURN
  END SUBROUTINE date_stamp

  FUNCTION date_(dd,mm,yyyy) RESULT (x)
! .. Implicit None Statement ..
    IMPLICIT NONE
! ..
! .. Function Return Value ..
    TYPE (date) :: x
! ..
! .. Scalar Arguments ..
    INTEGER, INTENT (IN) :: dd, mm, yyyy
! ..
    x = date(dd,mm,yyyy)
  END FUNCTION date_
```

```
  FUNCTION get_year(x)
! .. Implicit None Statement ..
    IMPLICIT NONE
! ..
! .. Function Return Value ..
    INTEGER :: get_year
! ..
! .. Structure Arguments ..
    TYPE (date), INTENT (IN) :: x
! ..
    get_year = x%year
  END FUNCTION get_year

  FUNCTION get_month(x)
! .. Implicit None Statement ..
    IMPLICIT NONE
! ..
! .. Function Return Value ..
    INTEGER :: get_month
! ..
! .. Structure Arguments ..
    TYPE (date), INTENT (IN) :: x
! ..
    get_month = x%month
  END FUNCTION get_month

  FUNCTION get_day(x)
! .. Implicit None Statement ..
    IMPLICIT NONE
! ..
! .. Function Return Value ..
    INTEGER :: get_day
! ..
! .. Structure Arguments ..
    TYPE (date), INTENT (IN) :: x
! ..
    get_day = x%day
  END FUNCTION get_day


END MODULE date_module
```

```
PROGRAM ch2611
! .. Use Statements ..
  USE date_module, ONLY : calendar_to_julian, &
     date, date_, &
     date_stamp, &
     date_to_day_in_year, &
     date_to_weekday_number, &
     get_day, &
     get_month, &
     get_year, &
     julian_to_date_and_week_and_day, &
     ndays, &
     year_and_day_to_date
! ..
! .. Implicit None Statement ..
  IMPLICIT NONE
! ..
! .. Local Scalars ..
  INTEGER :: dd, ddd, i, mm, ndiff, wd, yyyy
  CHARACTER (50) :: message
! ..
! .. Local Arrays ..
  INTEGER :: val(8)
! ..
! .. Intrinsic Functions ..
! compute date this year for changing clocks
! back to est.
! i.e.compute date for the last
! sunday in october for this year.
  INTRINSIC date_and_time
! ..
! .. Local Structures ..
  TYPE (date) :: date1, date2, x
! ..
! Test date_stamp
  message = ' date_stamp = '
  CALL date_stamp(message(15:))
  WRITE (*,'(a)') message
  message = ' date_stamp = '
  CALL date_stamp(message(15:),want_day=.FALSE.)
  WRITE (*,'(a)') message
```

```
   message = ' date_stamp = '
   CALL date_stamp(message(15:),short=.TRUE.)
   WRITE (*,'(a)') message
   message = ' date_stamp = '
   CALL date_stamp &
      (message(15:),want_day=.FALSE.,short=.TRUE.)
   WRITE (*,'(a)') message

   CALL date_and_time(values=val)

   yyyy = val(1)
   mm = 10

   DO i = 31, 26, -1
      x = date_(i,mm,yyyy)
      IF (date_to_weekday_number(x)==0) THEN
         PRINT *, 'turn clocks back to est on: '
         print *, i, ' october ', get_year(x)
         EXIT
      END IF
   END DO

! compute date this year for
! turning clocks ahead to dst
! i.e., compute date for the first
! sunday in april for this year.

   CALL date_and_time(values=val)

   yyyy = val(1)
   mm = 4

   DO i = 1, 8
      x = date_(i,mm,yyyy)
      IF (date_to_weekday_number(x)==0) THEN
         PRINT *, 'turn clocks ahead to dst on: '
         print *, i, ' april ', get_year(x)
         EXIT
      END IF
   END DO

   CALL date_and_time(values=val)
```

```
   yyyy = val(1)
   mm = 12
   dd = 31
   x = date_(dd,mm,yyyy)

!  is this a leap year? i.e., is
!  12/31/yyyy the 366th day of the year?

   IF (date_to_day_in_year(x)==366) THEN
     PRINT *, get_year(x), ' is a leap year'
   ELSE
     PRINT *, get_year(x), ' is not a leap year'
   END IF

   x = date_(1,1,1970)

   CALL julian_to_date_and_week_and_day &
     (calendar_to_julian(x),x,wd,ddd)

   IF (get_year(x)/=1970 .OR. &
     get_month(x)/=1 .OR. &
     get_day(x)/=1 .OR. &
     wd/=4 .OR. ddd/=1) THEN
     PRINT *, 'julian_to_date_and_week_and_day failed'
     print *,' date, wd, ddd = ', &
     get_year(x), get_month(x), get_day(x), wd, ddd
     STOP
   END IF

!  difference between to same
!  months and days over 1 leap year is 366.

   date1 = date_(22,5,1984)
   date2 = date_(22,5,1983)
   ndiff = ndays(date1,date2)
   yyyy = 1970
   x = year_and_day_to_date(yyyy,ddd)

   IF (ndiff/=366) THEN
     PRINT *, 'ndays failed; ndiff = ', ndiff
   ELSE
```

```
!    recover month and day
!    from year and day number.
     IF (get_month(x)/=1 .AND. get_day(x)/=1) THEN
        PRINT *, 'year_and_day_to_date failed'
        print *,' mma, dda = ', get_month(x), &
           get_day(x)
     ELSE
        PRINT *, '** date manipulation subroutines'
        print *, '** simple test ok.'
     END IF
   END IF


END PROGRAM ch2611
```

We also have an alternate form of array declaration in this program, which is given below. It is common in Fortran 77 style code:

```
   INTEGER :: val(8)
```

The next major addition to this code would be a date checking routine to test the validity of dates. This would be called from within our constructor date_. This would mean that we could never have an invalid date when using the date_module. This is left as a programming exercise.

26.12 Graphics example — dislin

The following is a rewrite of the earlier tsunami plotting program. It now uses a publically available graphics library called dislin. This is available from

- http://www.mps.mpg.de/dislin/

It is free for Linux operating systems. The tsunami plot can be found at

- http://www.kcl.ac.uk/fortran

There are some minor wrap problems with the code:

```
PROGRAM ch2612

USE DISLIN

   LOGICAL :: trial, screen
   REAL :: long, lat
   screen = .FALSE.
   trial = .FALSE.
```

```
   CALL datain(trial)

   PRINT *, ' Which region do you wish to plot?'
   PRINT *, ' 0 = all regions'
   PRINT *, ' 1 = Hawaii'
   PRINT *, ' 2 = New Zealand and South Pacific
Islands'
   PRINT *, ' 3 = Papua New Guinea and Solomon Islands'
   PRINT *, ' 4 = Indonesia'
   PRINT *, ' 5 = Philippines'
   PRINT *, ' 6 = Japan'
   PRINT *, ' 7 = Kuril Islands and Kamchatka'
   PRINT *, ' 8 = Alaska incluing Aleutian Islands'
   PRINT *, ' 9 = West Coast - North and Central
America'
   PRINT *, ' 10 = West Coast - South America'
120 READ (unit=*,fmt=*,end=130,err=130) nreg
130 IF ((nreg<0) .OR. (nreg>10)) THEN
     PRINT *, ' Please input a number between 0 and 10
inclusive'
     GO TO 120
   END IF

! dislin initialisation routines
! and setting of some basic components
! of the plot

! These are based on two program examples.

! Choose a file format

   CALL METAFL('PDF')

! da4l = din a4 landscape 2970*2100 points

   CALL SETPAG('DA4L')

! Initialise dislin

   CALL DISINI
```

```
! Plot a border round the page

  CALL PAGERA

! Choose font

  CALL PSFONT('HELVETICA')

! argument is the thickness of the frame in plot
coordinates.

  CALL FRAME(3)

! determines the position of an axis system.
! the lower left corner of the axis system

  CALL AXSPOS(400,1850)

! The size of the axis system
! are the length and height of an axis system in plot
coordinates. The default
! values are set to 2/3 of the page length and height.

  CALL AXSLEN(2400,1400)

! Define axis title

  CALL NAME('Longitude','X')

! Define axis title

  CALL NAME('Latitude','Y')

! This routine plots a title over an axis system.

  CALL TITLIN('Plot of 3034 Tsunami events ',3)

! determines which label types will be plotted on an
axis.
! MAP defines geographical labels which are plotted as
non negative floating-point
```

```
! numbers with the following characters 'W', 'E', 'N'
and 'S'.

   CALL LABELS('MAP','XY')

! plots a geographical axis system.

   CALL GRAFMP(-180.,180.,-180.,90.,-90.,90.,-90.,30.)

! The statement CALL GRIDMP (I, J) overlays an axis
system with a longitude
! and latitude grid where I and J are the number of
grid lines between labels in
! the X- and Y-direction.

   CALL GRIDMP(1,1)

! The routine WORLD plots coastlines and lakes.

   CALL WORLD

! The angle and height of the characters can be
changed with the routines AN-GLE
! and HEIGHT.

   CALL HEIGHT(50)

! This routine plots a title over an axis system. The
title may contain up to four lines of text

designated
! with TITLIN.

   CALL TITLE

! This is a call to the convert routine.
! This was required by UNIRAS
!   CALL convrt(trial)

! This is a call to the routine that actually plots
each event.
```

```
   CALL plotem(trial,nreg)

! DISFIN terminates DISLIN and prints a message on the
screen. The level is set back to 0.

   CALL DISFIN


END PROGRAM ch2612

SUBROUTINE datain(trial)

 COMMON /TSUNAM/ &
   reg0la(378) , &
   reg0lo(378) , &
   reg1la(206) , &
   reg1lo(206) , &
   reg2la(41) , &
   reg2lo(41) , &
   reg3la(54) , &
   reg3lo(54) , &
   reg4la(60) , &
   reg4lo(60) , &
   reg5la(1540) , &
   reg5lo(1540) , &
   reg6la(80) , &
   reg6lo(80) , &
   reg7la(144) , &
   reg7lo(144) , &
   reg8la(245) , &
   reg8lo(245) , &
   reg9la(285) , &
   reg9lo(285)

   LOGICAL :: trial
   CHARACTER (80) :: filnam

   IF (trial) THEN
     PRINT *, ' Entering data input phase'
   END IF
   filnam = 'tsunami.dat'
   OPEN (unit=50,file=filnam,err=100,status='OLD')
```

```
   GO TO 110
100 PRINT *, ' Error opening data file'
   PRINT *, ' Program terminates'
   STOP
110 DO i = 1, 378
      READ (unit=50,fmt=1000) reg0la(i), reg0lo(i)
   END DO
1000 FORMAT (1X,F7.2,2X,F7.2)
   DO i = 1, 206
      READ (unit=50,fmt=1000) reg1la(i), reg1lo(i)
   END DO
   DO i = 1, 41
      READ (unit=50,fmt=1000) reg2la(i), reg2lo(i)
   END DO
   DO i = 1, 54
      READ (unit=50,fmt=1000) reg3la(i), reg3lo(i)
   END DO
   DO i = 1, 60
      READ (unit=50,fmt=1000) reg4la(i), reg4lo(i)
   END DO
   DO i = 1, 1540
      READ (unit=50,fmt=1000) reg5la(i), reg5lo(i)
   END DO
   DO i = 1, 80
      READ (unit=50,fmt=1000) reg6la(i), reg6lo(i)
   END DO
   DO i = 1, 144
      READ (unit=50,fmt=1000) reg7la(i), reg7lo(i)
   END DO
   DO i = 1, 245
      READ (unit=50,fmt=1000) reg8la(i), reg8lo(i)
   END DO
   DO i = 1, 285
      READ (unit=50,fmt=1000) reg9la(i), reg9lo(i)
   END DO
   IF (trial) THEN
      DO i = 1, 10
         PRINT *, reg0la(i), '    ', reg0lo(i)
      END DO
      PRINT *, ' Exiting data input phase'
      READ *, dummy
   END IF
```

```
END SUBROUTINE datain

SUBROUTINE plotem(trial,nreg)

USE DISLIN

 COMMON /TSUNAM/ &
  reg0la(378) , &
  reg0lo(378) , &
  reg1la(206) , &
  reg1lo(206) , &
  reg2la(41) , &
  reg2lo(41) , &
  reg3la(54) , &
  reg3lo(54) , &
  reg4la(60) , &
  reg4lo(60) , &
  reg5la(1540) , &
  reg5lo(1540) , &
  reg6la(80) , &
  reg6lo(80) , &
  reg7la(144) , &
  reg7lo(144) , &
  reg8la(245) , &
  reg8lo(245) , &
  reg9la(285) , &
  reg9lo(285)

  LOGICAL :: trial
  INTEGER :: nreg
  INTEGER :: kolour=10
  DATA dwidth/1.0/

  IF (trial) THEN
    dwidth = 5.0
    PRINT *, ' Entering Plot points'
  END IF

  CALL INCMRK(-1)

  IF (nreg==0) THEN
```

```
    CALL SETCLR(kolour)
    CALL CURVMP(reg0lo,reg0la,378)
    kolour = kolour +30
    CALL SETCLR(kolour)
    CALL CURVMP(reg1lo,reg1la,206)
    kolour = kolour +30
    CALL SETCLR(kolour)
    CALL CURVMP(reg2lo,reg2la,41)
    kolour = kolour +30
    CALL SETCLR(kolour)
    CALL CURVMP(reg3lo,reg3la,54)
    kolour = kolour +30
    CALL SETCLR(kolour)
    CALL CURVMP(reg4lo,reg4la,60)
    kolour = kolour +30
    CALL SETCLR(kolour)
    CALL CURVMP(reg5lo,reg5la,1540)
    kolour = kolour +30
    CALL SETCLR(kolour)
    CALL CURVMP(reg6lo,reg6la,80)
    kolour = kolour +30
    CALL SETCLR(kolour)
    CALL CURVMP(reg7lo,reg7la,144)
    kolour = kolour +30
    CALL SETCLR(kolour)
    CALL CURVMP(reg8lo,reg8la,245)
    kolour = kolour +30
    CALL SETCLR(kolour)
    CALL CURVMP(reg9lo,reg9la,285)
  ELSE IF (nreg==1) THEN
    kolour = 10
    CALL SETCLR(kolour)
    CALL CURVMP(reg0lo,reg0la,378)
  ELSE IF (nreg==2) THEN
    kolour = 20
    CALL SETCLR(kolour)
    CALL CURVMP(reg1lo,reg1la,206)
  ELSE IF (nreg==3) THEN
    kolour = 30
    CALL SETCLR(kolour)
    CALL CURVMP(reg2lo,reg2la,41)
  ELSE IF (nreg==4) THEN
```

```
      kolour = 40
      CALL SETCLR(kolour)
      CALL CURVMP(reg3lo,reg3la,54)
   ELSE IF (nreg==5) THEN
      kolour = 50
      CALL SETCLR(kolour)
      CALL CURVMP(reg4lo,reg4la,60)
   ELSE IF (nreg==6) THEN
      kolour = 60
      CALL SETCLR(kolour)
      CALL CURVMP(reg5lo,reg5la,1540)
   ELSE IF (nreg==7) THEN
      kolour = 70
      CALL SETCLR(kolour)
      CALL CURVMP(reg6lo,reg6la,80)
   ELSE IF (nreg==8) THEN
      kolour = 80
      CALL SETCLR(kolour)
      CALL CURVMP(reg7lo,reg7la,144)
   ELSE IF (nreg==9) THEN
      kolour = 90
      CALL SETCLR(kolour)
      CALL CURVMP(reg8lo,reg8la,245)
   ELSE IF (nreg==10) THEN
      kolour = 100
      CALL SETCLR(kolour)
      CALL CURVMP(reg9lo,reg9la,285)
   END IF
   IF (trial) THEN
      PRINT *, ' Exiting Plot points'
   END IF

END SUBROUTINE plotem
```

26.13 Problems

1. Compile and run ch2606. Try running it with matrices of your own choice.

2. Write a generic subroutine Swap which two takes arguments a and b (real or integer) and swaps them. Write a main program that reads two real values and calls Swap and then reads two integer values and again calls Swap.

3. Using ch2605 as a starting point extend the program to overload the subtraction operator (–), for the user defined type position.

4. Modify the elemental function example to include usage of the function etox with a rank 2 or higher array. Also add a call to the intrinsic function exp and compare the results.

5. Using the balanced tree example as a basis and modify it to work with a character array rather than an integer. The routine that prints the tree will also have to be modified to reflect this.

6. Compile and run the program that calculated the inner product of two sparse vectors using the data supplied. This should produce the answer 19.

26.14 Bibliography

Duff I.S., Erismon A.M., Reid J.K., *Direct Methods for Sparse Matrices*, Oxford Science Publications, 1986.

- Authoritative coverage of this area. Relatively old, but well regarded. Code segments and examples are a mixture of Fortran 77 and Algol 60 (which of course do not support pointers) and therefore the implementation of linked lists is done using the existing features of these languages. The onus is on the programmer to correctly implement linked lists using fixed size arrays rather than using the features provided by pointers in a language. It is remarkable how elegant these solutions are, given the lack of dynamic data structures in these two languages.

Hopkins T., Phillips C., *Numerical Methods in Practice, Using the NAG Library*. Addison-Wesley, 1988.

- Good adjunct to the NAG library documentation for the less numerate user.

Schneider G.M., Bruell S.C., *Advanced Programming and Problem Solving with Pascal,* Wiley, 1981.

- The book is aimed at computer science students and follows the curriculum guidelines laid down in *Communications of the ACM*, August 1985, Course CS2. The book is very good for the complete beginner as the examples are very clearly laid out and well explained. There is a coverage of data structures, abstract data types and their implementation, algorithms for sorting and searching, the principles of software development as they relate to the specification, design, implementation and verification of programs in an orderly and disciplined fashion — their words.

Vowels R.A., *Algorithms and Data Structures in F and Fortran,* Unicomp, 1998.

- The only book currently that uses Fortran 90/95 and F. Visit the Fortran web site for more details. They are the publishers.

- http://www.fortran.com/fortran/market.html

Wirth N., *Algorithms + Data Structures = Programs*, Prentice-Hall, 1976.

- An early but illuminating book on the subject. Well worth a read. Pascal is used.

Wirth N., *Algorithms + Data Structures*, Prentice-Hall, 1986.

- This is the Modula 2 version. Closer to Fortran than the Pascal version.

27

ISO TR 15580 IEEE Arithmetic

"'Can you do addition?' the White Queen asked. 'What's one and one and one and one and one and one and one and one and one and one?"'

'I don't know,' said Alice. 'I lost count.'

Lewis Carroll, *Through the Looking Glass and What Alice Found There*

Aims

The aims of this chapter are to look in more depth at arithmetic and in particular at the support that Fortran provides for the IEEE 754 standard. There is a coverage of:

- Hardware support for arithmetic.
- Integer formats.
- Floating point formats: single and double.
- Special values: denormal, infinity and not a number — NAN.
- Exceptions and flags: divide by zero, inexact, invalid, overflow, underflow.

27 ISO TR 15580 — IEEE Arithmetic

The literature contains details of the IEEE 754 standard and the bibliography contains details of a number of printed and on-line sources.

27.1 History

When we use programming languages to do arithmetic two major concerns are the ability to develop reliable **and** portable numerical software. Arithmetic is done in hardware and there are a number of things to consider:

- The range of hardware available both now and in the past.
- The evolution of hardware.

There has been a very considerable change in arithmetic units since the first computers. The following is a list of hardware and computing systems that the authors have some used or have heard of. It is not exhaustive or definitive, but rather reflects the authors' age and experience:

- CDC
- Cray
- IBM
- ICL
- Fujitsu
- DEC
- Compaq
- Gateway
- Sun
- Silicon Graphics
- Hewlett Packard
- Data General
- Honeywell
- Elliot
- Mostek
- National Semiconductors
- Intel

- Zilog
- Motorola
- Signetics
- Amdahl
- Texas Instruments
- Cyrix

Some of the operating systems include:

- NOS
- NOS/BE
- Kronos
- UNIX
- VMS
- Dos
- Windows 3.x
- Windows 95
- Windows 98
- Windows NT
- Windows 2000
- MVS
- VM
- CP/M
- Macintosh
- OS/2

Again the list is not exhaustive or definitive. The intention is simply to provide some idea of the wide range of hardware, computer manufacturers and operating systems that have been around in the past 50 years.

To cope with the anarchy in this area Doctor Robert Stewart (acting on behalf of the IEEE) convened a meeting which led to the birth of IEEE 754.

The first draft, which was prepared by William Kahan, Jerome Coonen and Harold Stone, was called the KCS draft and eventually adopted as IEEE 754. A fascinat-

ing account of the development of this standard can be found in *An Interview with the Old Man of Floating Point*, and the bibliography provides a web address for this interview. Kahan went on to get the ACM Turing Award in 1989 for his work in this area.

This has become a de facto standard amongst arithmetic units in modern hardware. Note that it is not possible to describe precisely the answers a program will give, and the authors of the standard knew this. This goal is virtually impossible to achieve when one considers floating point arithmetic. Reasons for this include:

- The conversions of numbers between decimal and binary formats.
- The use of elementary library functions.
- Results of calculations may be in hardware inaccessible to the programmer.
- Intermediate results in subexpressions or arguments to procedures.

The bibliography contains details of a paper that addresses this issue in much greater depth — *Differences Among IEEE 754 Implementations.*

Fortran is one of a small number of languages that provides access to IEEE arithmetic, and it achieves this via TR1880 which is an integral part of Fortran 2003. The C standard (C9X) addresses this issue and Java offers limited IEEE arithmetic support. More information can be found in the references at the end of the chapter.

27.2 IEEE 754 Specifications

The standard specifies a number of things including:

- Single precision floating point format.
- Double precision floating point format.
- Two classes of extended floating point formats.
- Accuracy requirements on the following floating point operations:
  - Add.
  - Subtract.
  - Multiply.
  - Divide.
  - Square root.
  - Remainder.
  - Round numbers in floating point format to integer values.

    - Convert between different floating point formats.
    - Convert between floating point and integer format.
    - Compare.
- Base conversion, i.e., when converting between decimal and binary floating point formats and vice versa.
- Exception handling for:
    - Divide by zero.
    - Overflow.
    - Underflow.
    - Invalid operation.
    - Inexact.
- Rounding directions.
- Rounding precisions.

We will look briefly at each of these requirements.

27.2.1 Single precision floating point format

This is a 32-bit quantity made up of a sign bit, 8-bit biased exponent and 23-bit mantissa. The standard also specifies that certain of the bit patterns are set aside and do not represent normal numbers. This means that valid numbers are in the range 3.40282347E+38 to 1.17549435E-38 and the precision is between 6 and 9 digits depending on the numbers.

The special bit patterns provide the following:

- +0
- -0
- subnormal numbers in the range 1.17549421E-38 to 1.40129846E-45
- + infinity
- - infinity
- quiet NaN (Not a Number)
- signalling NaN

One of the first systems that the authors worked with that had special bit patterns set aside was the CDC 6000 range of computers that had negative indefinite and infinity. Thus the ideas are not new, as this was in the late 1970s.

The support of positive and negative zero means that certain problems can be handled correctly including:

- The evaluation of the log function which has a discontinuity at zero.
- The equation $\sqrt{1/z} = 1/\sqrt{z}$ can be solved when $z = -1$.

See also the Kahan paper *Branch Cuts for Complex Elementary Functions, or Much Ado About Nothing's Sign Bit* for more details.

Subnormals, which permit gradual underflow, fill the gap between 0 and the smallest normal number.

Simply stated underflow occurs when the result of an arithmetic operation is so small that it is subject to a larger than normal rounding error when stored. The existence of subnormals means that greater precision is available with these small numbers than with normal numbers. The key features of gradual underflow are:

- When underflow does occur there should never be a loss of accuracy any greater than that from ordinary roundoff.
- The operations of addition, subtraction, comparison and remainder are always exact.
- Algorithms written to take advantage of subnormal numbers have smaller error bounds than other systems.
- If x and y are within a factor of 2 then x-y is error free, which is used in a number of algorithms that increase the precision at critical regions.

The combination of positive and negative zero and subnormal numbers means that when x and y are small and x-y has been flushed to zero the evaluation of

- $1/(x-y)$

can be flagged and located.

Certain arithmetic operations cause problems including:

- $0 * \infty$
- $0 / 0$
- $\sqrt{x}$ when $x < 0$

and the support for NaN handles these cases.

The support for positive and negative infinity allows the handling of

- $x / 0$ when x is nonzero and of either sign

and the outcome of this means that we write our programs to take the appropriate action. In some cases this would mean recalculating using another approach.

For more information see the references in the bibliography.

27.2.2 Double precision floating point format

This is a 64-bit quantity made up of a sign bit, 11-bit biased exponent and 52-bit mantissa. As with single precision the standard specifies that certain of the bit patterns are set aside and do not represent normal numbers. This means we have valid numbers in the range 1.7976931348623157E308 to 2.2250738585072014E-308 and precision between 15 and 17 digits depending on the numbers.

As with single precision there are bit patterns set aside for the same special conditions.

Note that this does not mean that the hardware has to handle the manipulation of this 64-bit quantity in an identical fashion. The Sparc and Intel family handle the above as two 32-bit quantities but the order of the two component parts is reversed — so-called big endian and little endian.

27.2.3 Two classes of extended floating point formats

These formats are not mandatory. A number of variants of double extended exist including:

- Sun — four 32-bit words, one sign bit, 15-bit biased exponent and 112-bit mantissa, numbers in the range 3.362E-4932 to 1.189E4932, 33–36 digits of significance.
- Intel — 10 bytes — one sign bit, 15-bit biased exponent, 63-bit mantissa, numbers in the range 3.362E-4932 to 1.189E4932, 18–21 digits of significance.
- PowerPC — as Sun.

27.2.4 Accuracy requirements

Remainder and compare must be exact. The rest should return the exact result if possible. If not, there are well-defined rounding rules to apply.

27.2.5 Base conversion — Converting between decimal and binary floating point formats and vice versa

These results should be exact if possible; if not the results must differ by tolerances that depend on the rounding mode.

27.2.6 Exception handling

It must be possible to signal to the user the occurrence of the following conditions or exceptions:

- Divide by zero.
- Overflow.
- Underflow.
- Invalid operation.
- Inexact.

The ability to detect the above is a big step forward in our ability to write robust and portable code. These operations do occur in calculations and it is essential to have user programmer control over what action to take.

27.2.7 Rounding directions

Four rounding directions are available:

- Nearest — the default.
- Down.
- Up.
- Chop.

Access to directed rounding can be used to implement interval arithmetic, for example.

27.2.8 Rounding precisions

The only mandatory part here is that machines that perform computations in extended mode let the programmer control the precision via a control word. This means that if software is being developed on machines that support extended modes those machines can be switched to a mode that would enable the software to run on a system that didn't support extended modes. This area looks like a can of worms. Look at the Kahan paper for more information — *Lecture Notes on the Status of IEEE 754*.

27.3 Resumé

The above has provided a quick tour of IEEE 754. We'll now look at what Fortran has to offer to support it.

27.4 ISO TR 15580

Fortran provides access to the facilities via the USE statement. The current standard does not have the concept of an intrinsic module. TR 15580 introduces this concept. Three modules are provided:

- ieee_features
- ieee_exceptions
- ieee_arithmetic

The first thing to consider is the degree of conformance to the IEEE standard. It is possible that not all of the features are supported. Thus the first thing to do is to run one or more test programs to determine the degree of support for a particular system.

27.4.1 IEEE_FEATURES module

This module defines a derived type, IEEE_FEATURES_TYPE, and up to 11 constants of that type representing IEEE features:

- IEEE_DATATYPE — whether any IEEE data types are available.
- IEEE_DENORMAL — whether IEEE denormal values are available.
- IEEE_DIVIDE — whether division has the accuracy required by IEEE.
- IEEE_HALTING — whether control of halting is supported.
- IEEE_INEXACT_FLAG — whether the inexact exception is supported.
- IEEE_INF — whether IEEE positive and negative infinities are available.
- IEEE_INVALID_FLAG — whether the invalid exception is supported.
- IEEE_NAN — whether IEEE NaNs are available.
- IEEE_ROUNDING — whether all IEEE rounding modes are available.
- IEEE_SQRT — whether SQRT conforms to the IEEE standard.
- IEEE_UNDERFLOW_FLAG — whether underflow is supported.

27.4.2 IEEE_EXCEPTIONS module

This module provides data types, constants and generic procedures for IEEE exceptions:

TYPE IEEE_STATUS_TYPE

Variables of this type can hold a floatingpoint status value.

SUBROUTINE IEEE_GET_STATUS(STATUS_VALUE)

TYPE(IEEE_STATUS_TYPE),INTENT(OUT) :: STATUS_VALUE

Stores the current floatingpoint status into the STATUS_VALUE argument.

SUBROUTINE IEEE_SET_STATUS(STATUS_VALUE)

TYPE(IEEE_STATUS_TYPE),INTENT(IN) :: STATUS_VALUE

Sets the current floatingpoint status from the STATUS_VALUE argument.

TYPE IEEE_FLAG_TYPE

Values of this type specify individual IEEE exception flags; constants for these are available as follows:

TYPE(IEEE_FLAG_TYPE),PARAMETER :: IEEE_DIVIDE_BY_ZERO

TYPE(IEEE_FLAG_TYPE),PARAMETER :: IEEE_INEXACT

TYPE(IEEE_FLAG_TYPE),PARAMETER :: IEEE_INVALID

TYPE(IEEE_FLAG_TYPE),PARAMETER :: IEEE_OVERFLOW

TYPE(IEEE_FLAG_TYPE),PARAMETER :: IEEE_UNDERFLOW

In addition, two array constants are available for indicating common combinations of flags:

TYPE(IEEE_FLAG_TYPE),PARAMETER :: &

IEEE_USUAL(3) = (/&

IEEE_DIVIDE_BY_ZERO,&

IEEE_INVALID, &

IEEE_OVERFLOW /), &

IEEE_ALL(5) = (/&

IEEE_DIVIDE_BY_ZERO,&

IEEE_INEXACT, &

IEEE_INVALID,&

IEEE_OVERFLOW, &

IEEE_UNDERFLOW /)

LOGICAL FUNCTION IEEE_SUPPORT_FLAG(FLAG,X)

TYPE(IEEE_FLAG_TYPE),INTENT(IN) :: FLAG

REAL(kind),INTENT(IN),OPTIONAL :: X

Returns TRUE if detection of the specified IEEE exception is supported for the REAL kind of X (if X is present), or for all REAL kinds (if X is absent).

LOGICAL FUNCTION IEEE_SUPPORT_HALTING(FLAG)

TYPE(IEEE_FLAG_TYPE),INTENT(IN) :: FLAG

Returns TRUE if IEEE_SET_HALTING_MODE can be used to change whether the processor terminates the program on receiving the specified exception.

ELEMENTAL SUBROUTINE &
IEEE_GET_FLAG(FLAG,FLAG_VALUE)

TYPE(IEEE_FLAG_TYPE),INTENT(IN) :: FLAG

LOGICAL,INTENT(OUT) :: FLAG_VALUE

Sets (each element of) FLAG_VALUE to TRUE if the corresponding exception specified by FLAG is signalling, and to FALSE otherwise.

ELEMENTAL SUBROUTINE &
IEEE_GET_HALTING_MODE(FLAG,HALTING)

TYPE(IEEE_FLAG_TYPE),INTENT(IN) :: FLAG

LOGICAL,INTENT(OUT) :: HALTING

Sets (each element of) HALTING to TRUE if the corresponding exception specified by FLAG is signalling, and to FALSE otherwise.

ELEMENTAL SUBROUTINE IEEE_SET_FLAG(FLAG,FLAG_VALUE)

TYPE(IEEE_FLAG_TYPE),INTENT(OUT) :: FLAG

LOGICAL,INTENT(IN) :: FLAG_VALUE

Sets the exception flag specified by (each element of) FLAG to signalling or quiet according to the corresponding element of FLAG_VALUE.

ELEMENTAL SUBROUTINE &
IEEE_SET_HALTING_MODE(FLAG,HALTING)

TYPE(IEEE_FLAG_TYPE),INTENT(OUT) :: FLAG

LOGICAL,INTENT(IN) :: HALTING

Sets the halting mode for each exception specified by FLAG to the value of the corresponding element of HALTING (TRUE = halt).

27.4.3 IEEE_ARITHMETIC module

These are given below:

27.4.3.1 IEEE data type selection

INTEGER FUNCTION SELECTED_REAL_KIND(P,R)

INTEGER(kind1),OPTIONAL :: P

INTEGER(kind2),OPTIONAL :: R

The same as the SELECTED_REAL_KIND intrinsic, but only returns information about the IEEE kinds of reals.

27.4.3.2 General support enquiry functions

LOGICAL FUNCTION IEEE_SUPPORT_DATATYPE(X)

REAL(kind),OPTIONAL :: X

Whether IEEE arithmetic is supported for the same kind of REAL as X (or for all REAL kinds if X is absent).

LOGICAL FUNCTION IEEE_SUPPORT_DENORMAL(X)

REAL(kind),OPTIONAL :: X

Whether IEEE denormal values are supported for the same kind of REAL as X (or for all REAL kinds if X is absent).

LOGICAL FUNCTION IEEE_SUPPORT_DIVIDE(X)

REAL(kind),OPTIONAL :: X

Whether division is carried out to the accuracy specified by the IEEE standard for the same kind of REAL as X (or for all REAL kinds if X is absent).

LOGICAL FUNCTION IEEE_SUPPORT_INF(X)

REAL(kind),OPTIONAL :: X

Whether IEEE infinite values are supported for the same kind of REAL as X (or for all REAL kinds if X is absent).

LOGICAL FUNCTION IEEE_SUPPORT_NAN(X)

REAL(kind),OPTIONAL :: X

Whether IEEE NaN (Not-a-Number) values are supported for the same kind of REAL as X (or for all REAL kinds if X is absent).

LOGICAL FUNCTION IEEE_SUPPORT_SQRT(X)

REAL(kind),OPTIONAL :: X

Whether SQRT conforms to the IEEE standard for the same kind of REAL as X (or for all REAL kinds if X is absent).

LOGICAL FUNCTION IEEE_SUPPORT_STANDARD(X)

REAL(kind),OPTIONAL :: X

Whether all the IEEE facilities specified by the TR are supported for the same kind of REAL as X (or for all REAL kinds if X is absent).

27.4.3.3 Rounding modes

TYPE IEEE_ROUND_TYPE

Values of this type specify the IEEE rounding mode.

TYPE (IEEE_ROUND_TYPE) , &
PARAMETER :: IEEE_DOWN

TYPE (IEEE_ROUND_TYPE) , &
PARAMETER :: IEEE_NEAREST

TYPE (IEEE_ROUND_TYPE) ,
PARAMETER :: IEEE_TO_ZERO

TYPE (IEEE_ROUND_TYPE) , PARAMETER :: IEEE_UP

LOGICAL FUNCTION IEEE_SUPPORT_ROUNDING(ROUND_VALUE,X)

TYPE(IEEE_ROUND_TYPE),INTENT(IN) :: ROUND_VALUE

REAL(kind),OPTIONAL :: X

Whether the specified IEEE rounding mode is supported for the same kind of REAL as X (or for all REAL kinds if X is absent).

SUBROUTINE IEEE_GET_ROUNDING_MODE(ROUND_VALUE)

TYPE(IEEE_ROUND_TYPE),INTENT(OUT) :: ROUND_VALUE

Sets the ROUND_VALUE argument to the current IEEE rounding mode.

SUBROUTINE IEEE_SET_ROUNDING_MODE(ROUND_VALUE)

TYPE (IEEE_ROUND_TYPE) , INTENT(IN) :: ROUND_VALUE

Sets the current IEEE rounding mode to that specified by ROUND_VALUE.

27.4.3.4 Number classification

TYPE IEEE_CLASS_TYPE

Values of this type indicate the IEEE class of a number.

TYPE (IEEE_CLASS_TYPE) , &
PARAMETER :: IEEE_NEGATIVE_DENORMAL

TYPE (IEEE_CLASS_TYPE) , PARAMETER :: IEEE_NEGATIVE_INF

TYPE (IEEE_CLASS_TYPE) , PARAMETER :: IEEE_NEGATIVE_NORMAL

TYPE (IEEE_CLASS_TYPE) , PARAMETER :: IEEE_NEGATIVE_ZERO

TYPE (IEEE_CLASS_TYPE) , PARAMETER :: IEEE_POSITIVE_DENORMAL

TYPE (IEEE_CLASS_TYPE) , PARAMETER :: IEEE_POSITIVE_INF

TYPE(IEEE_CLASS_TYPE) , PARAMETER :: IEEE_POSITIVE_NORMAL

TYPE(IEEE_CLASS_TYPE) , PARAMETER :: IEEE_POSITIVE_ZERO

TYPE(IEEE_CLASS_TYPE) , PARAMETER :: IEEE_QUIET_NAN

TYPE(IEEE_CLASS_TYPE) , PARAMETER :: IEEE_signalling_NAN

ELEMENTAL TYPE(IEEE_CLASS_TYPE) FUNCTION IEEE_CLASS(X)

REAL(kind),INTENT(IN) :: X

Returns the appropriate value of IEEE_CLASS_TYPE for the number X, which may be of any IEEE kind.

In addition to ISO/IEC TR 15580:1998(E), the module IEEE_ARITHMETIC defines the "==" and "/=" operators for the IEEE_CLASS_TYPE. These may be used to test the return value of the IEEE_CLASS function, e.g.,

```
USE,INTRINSIC :: IEEE_ARITHMETIC, ONLY: IEEE_CLASS, &
IEEE_QUIET_NAN, OPERATOR(==)
 ...
IF (IEEE_CLASS(X)==IEEE_QUIET_NAN) THEN
  ...
```

ELEMENTAL REAL(kind) FUNCTION IEEE_VALUE(X,CLASS)

REAL(kind),INTENT(IN) :: X

TYPE(IEEE_CLASS_TYPE),INTENT(IN) :: CLASS

Returns a sample value of the specified class for the same kind of real as X, which may be of any IEEE kind.

ELEMENTAL LOGICAL FUNCTION IEEE_IS_FINITE(X)

REAL(kind),INTENT(IN) :: X

Returns TRUE if X is not infinite or NaN.

ELEMENTAL LOGICAL FUNCTION IEEE_IS_NAN(X)

REAL(kind),INTENT(IN) :: X

Returns TRUE if X is either a signalling or quiet NaN.

ELEMENTAL LOGICAL FUNCTION IEEE_IS_NEGATIVE(X)

REAL(kind),INTENT(IN) :: X

Returns TRUE if X is negative, including negative zero.

ELEMENTAL LOGICAL FUNCTION IEEE_IS_NORMAL(X)

REAL(kind),INTENT(IN) :: X

Returns TRUE if X is not an infinity, NaN, or denormal.

ELEMENTAL LOGICAL FUNCTION IEEE_UNORDERED(X,Y)

REAL(kind),INTENT(IN) :: X,Y

Returns TRUE if X is a NaN or if Y is a NaN.

27.4.3.5 Arithmetic operations

ELEMENTAL REAL(kind) FUNCTION IEEE_COPY_SIGN(X,Y)

REAL (kind) , INTENT(IN) :: X,Y

Returns X with the sign of Y, even for NaNs and infinities.

ELEMENTAL REAL (kind) FUNCTION IEEE_LOGB(X)

REAL (kind) , INTENT(IN) :: X

Returns the unbiased exponent as a REAL value:

If X is zero, IEEE_DIVIDE_BY_ZERO signals and the result is –infinity if IEEE infinities are supported for that kind, and –HUGE(X) if not.

If X is infinite, the result is +infinity.

If X is a NaN, the result is a quiet NaN (the same one if X is a quiet NaN); otherwise the result is EXPONENT(X)-1.

ELEMENTAL REAL (kind) FUNCTION IEEE_NEXT_AFTER(X,Y)

REAL (kind) , INTENT(IN) :: X,Y

The same as NEAREST(X,1.0_kind) for Y>X and NEAREST(X,-1.0_kind) for Y<X; if Y==X, the result is X, if either X or Y are NaNs the result is one of these NaNs.

ELEMENTAL REAL (kind) FUNCTION IEEE_REM(X,Y)

REAL (kind) , INTENT(IN) :: X,Y

X-Y*N exactly, where N is the integer nearest to the exact value X/Y. If the result is zero, it has the same sign as X. This function is not affected by the rounding mode.

ELEMENTAL REAL (kind) FUNCTION IEEE_RINT(X)

REAL (kind) , INTENT(IN) :: X

Round to an integer according to the current rounding mode.

ELEMENTAL REAL (kind) FUNCTION IEEE_SCALB(X,I)

REAL (kind1) , INTENT(IN) :: X

INTEGER (kind2) , INTENT(IN) :: I

The same as SCALE(X,I).

27.5 Summary

Support for the above is relatively limited at the time of writing this book. There is always a time lag between the formal publication of a standard and the implementation in production compilers. As compiler support improves examples will be added to our web site. Our home page is:

- http://www.kcl.ac.uk/fortran

27.6 Bibliography

Hauser J.R., Handling Floating Point Exceptions in Numeric Programs, *ACM Transaction on Programming Languages and Systems*, Vol. 18, No. 2, March 1996, pp. 139–174.

- The paper looks at a number of techniques for handling floating point exceptions in numeric code. One of the conclusions is for better structured support for floating point exception handling in new programming languages, or of course better standards for existing languages.

IEEE, *IEEE Standard for Binary Floating-Point Arithmetic, ANSI/IEEE Std 754-1985*, Institute of Electrical and Electronic Engineers Inc.

- The formal definition of IEEE 754.

Knuth D., *Seminumerical Algorithms*, Addison-Wesley, 1969.

- There is a coverage of floating point arithmetic, multiple precision arithmetic, radix conversion and rational arithmetic.

Sun, *Numerical Computation Guide*, SunPro.

- Very good coverage of the numeric formats for IEEE Standard 754 for Binary Floating-Point Arithmetic. All SunPro compiler products support the features of the IEEE 754 standard.

27.6.1 Web-based sources

http://validgh.com/goldberg/addendum.html

- *Differences Among IEEE 754 Implementations.* The material in this paper will eventually be included in the Sun Numerical Computation Guide as an addendum to Appendix D, David Goldberg's *What Every Computer Scientist Should Know about Floating Point Arithmetic.*

http://docs.sun.com/

- Follow the links to the *Floating Point and Common Tools AnswerBook*. The *Numerical Computation Guide* can be browsed on-line or downloaded as a pdf file. The last time we checked it was about 260 pages. Good source of information if you have Sun equipment.

http://www.validgh.com/

- This web site contains technical and business information relating to the validgh professional consulting practice of David G. Hough. Contains links to the Goldberg paper and the above addendum by Doug Priest.

http://babbage.cs.qc.edu/courses/cs341/IEEE-754references.html

- Brief coverage of IEEE arithmetic with pointers to further sources. There is also a coverage of the storage layout and ranges of floating point numbers. Computer Science 341 is an introduction to the design of a computer's hardware, particularly the CPU and memory systems.

http://www.nag.co.uk/nagware/NP/TR.html

- NAG provide coverage of TR 15580 and TR 15581. The first is the support Fortran has for IEEE arithmetic.

http://www.cs.berkeley.edu/~wkahan/

- Willam Kahan home page.

http://www.cs.berkeley.edu/~wkahan/ieee754status/754story.html

- An Interview with the Old Man of Floating Point. Reminiscences elicited from William Kahan by Charles Severance, which appeared in an issue of *IEEE Computer* - March 1998.

http://www.cs.berkeley.edu/~wkahan/ieee754status/ieee754.ps

- Lecture Notes on the Status of IEEE Standard 754 for Binary Floating-Point Arithmetic. Well worth a read.

http://www.stewart.cs.sdsu.edu/cs575/labs/l3floatpt.html

- *CS 575 Supercomputing — Lab 3: Floating Point Arithmetic.* CS 575 is an interdisciplinary course to introduce students in the sciences and engineering to advanced computing techniques using the supercomputers at the San Diego Supercomputer Center (SDSC).

http://www.mathcom.com/nafaq/index.html

- *FAQ: Numerical Analysis and Associated Fields Resource Guide*. A summary of Internet resources for a number of fields related to numerical analysis.

http://www.math.psu.edu/dna/disasters/ariadne.html

- *The Explosion of the Ariane 5*: A 64-bit floating point number relating to the horizontal velocity of the rocket with respect to the platform was converted to a 16-bit signed integer. The number was larger than 32,768, the largest integer storeable in a 16-bit signed integer, and thus the conversion failed.

27.6.2 Hardware sources

Osbourne A., Kane G., *4-bit and 8-bit Microprocessor Handbook,* Osbourne/McGraw-Hill, 1981.

- Good source of information on 4-bit and 8-bit microprocessors.

Osbourne A., Kane G., *16-Bit Microprocessor Handbook,* Osbourne/McGraw-Hill, 1981.

- Ditto 16-bit microprocessors.

Intel, *386 DX Microprocessor Hardware Reference Manual*, Intel.

- The first Intel offering with 32-bit addressing.

Intel, *80386 System Software Writer's Guide,* Intel.

- Developer's guide to the above.

http://www.intel.com/

- Intel's home page.

http://developer.intel.com/design/pentiumiii/

- Details of the Pentium III processor.

http://www.cyrix.com/

- Cyrix home page.

Bhandarkar D.P., *Alpha Implementations and Architecture: Complete Reference and Guide,* Digital Press, 1996.

- Looks at some of the trade-offs and design philosophy behind the alpha chip. The author worked with VAX, MicroVAX and VAX vectors as well as the Prism. Also looks at the GEM compiler technology that DEC/Compaq use.

http://www.digital.com/alphaserver/workstations/

- Home page for the Compaq/DEC Alpha systems.

http://www.sgi.com/

- Silicon Graphics home page.

http://www.sun.com/

- Sun home page.

http://www.ibm.com/

- IBM home page.

27.6.3 Operating Systems

Deitel H.M., *An Introduction to Operating Systems*, Addison-Wesley, 1990.

- The revised first edition includes case studies of UNIX, VMS, CP/M, MVS and VM. The second edition adds OS/2 and the Macintosh operating systems. There is a coverage of hardware, software, firmware, process management, process concepts, asynchronous concurrent processes, concurrent programming, deadlock and indefinite postponement, storage management, real storage, virtual storage, processor management, distributed computing, disk performance optimisation, file and database systems, performance, coprocessors, risc, data flow, analytic modelling, networks, security and it concludes with case studies of the these operating systems. The book is well written and an easy read.

27.6.4 Java and IEEE 754

http://www.cs.berkeley.edu/~darcy/Borneo/

- *Borneo Language Homepage*: Borneo is a dialect of the Java language designed to have true support for the IEEE 754 floating point standard. The status of arithmetic in Java is fluid. At the time of writing this book Sun had withdrawn from the formal language standardisation process. Sun

have a publication at their web site that addresses changes to the Java language specification for JDK Release 1.2 floating point arithmetic. Their home Java page is

- http://www.java.sun.com/

27.6.5 C and IEEE 754

http://wwwold.dkuug.dk/JTC1/SC22/WG14/

- The official home of JTC1/SC22/WG14 - C. The C programming language standard ISO/IEC 9899 was adopted by ISO in 1990. ANSI then replaced their first standard X3.159 by the ANSI/ISO 9899 standard identical to ISO/IEC 9899:1990.

28

ISO TR 15581 Allocatable Enhancements

Aim

The aim of this chapter is to provide a small number of examples illustrating some of the features introduced with ISO TR 15581:

- Allocatable dummy arrays.
- Allocatable function results.
- Allocatable structure components.

28 ISO TR 15581 Allocatable Enhancements

In this chapter we provide three examples that illustrate the features introduced by TR 15581. The facilities mean that we do not have to use pointers and this has several efficiency benefits as the compiler does not have to worry about aliasing and whether it can deallocate temporaries or not. There is also the issue of contiguous memory allocation for allocatable arrays, which can't be guaranteed when using pointers and sections and strides other than unity.

28.1 Allocatable dummy array example

In the Quicksort example the actual array allocation took place in the main program. In this example we do the allocation in the Read_Data subroutine:

```
PROGRAM ch2801
IMPLICIT NONE
INTEGER :: How_Many
CHARACTER (LEN=20) :: File_Name
REAL , ALLOCATABLE , DIMENSION(:) :: Raw_Data
integer , dimension(8) :: timing

INTERFACE
  SUBROUTINE Read_Data(File_Name,Raw_Data,How_Many)
    IMPLICIT NONE
    CHARACTER (LEN=*) , INTENT(IN) :: File_Name
    INTEGER , INTENT(IN) :: How_Many
    REAL , INTENT(OUT) , ALLOCATABLE , &
    DIMENSION(:) :: Raw_Data
  END SUBROUTINE Read_Data
END INTERFACE

INTERFACE
  SUBROUTINE Sort_Data(Raw_Data,How_Many)
    IMPLICIT NONE
    INTEGER , INTENT(IN) :: How_Many
    REAL , INTENT(INOUT) , DIMENSION(:) :: Raw_Data
  END SUBROUTINE Sort_Data
END INTERFACE

INTERFACE
  SUBROUTINE Print_Data(Raw_Data,How_Many)
    IMPLICIT NONE
    INTEGER , INTENT(IN) :: How_Many
```

```
      REAL , INTENT(IN) , DIMENSION(:) :: Raw_Data
   END SUBROUTINE Print_Data
END INTERFACE
   PRINT * , ' How many data items are there?'
   READ  * , How_Many
   PRINT * , ' What is the file name?'
   READ '(A)',File_Name
   call date_and_time(values=timing)
   print * , ' initial'
   print * , timing(6),timing(7),timing(8)
   CALL Read_Data(File_Name,Raw_Data,How_Many)
   call date_and_time(values=timing)
   print * , ' read and allocate'
   print * , timing(6),timing(7),timing(8)
   CALL Sort_Data(Raw_Data,How_Many)
   call date_and_time(values=timing)
   print * , ' sort'
   print * , timing(6),timing(7),timing(8)
   CALL Print_Data(Raw_Data,How_Many)
   call date_and_time(values=timing)
   print * , ' print'
   print * , timing(6),timing(7),timing(8)
   PRINT * , ' '
   PRINT *, ' Data written to file SORTED.DAT'

END PROGRAM ch2801

SUBROUTINE Read_Data(File_Name,Raw_Data,How_Many)
IMPLICIT NONE
CHARACTER (LEN=*) , INTENT(IN) :: File_Name
INTEGER , INTENT(IN) :: How_Many
REAL , INTENT(OUT) , ALLOCATABLE , &
   DIMENSION(:) :: Raw_Data

INTEGER :: I
   ALLOCATE(Raw_Data(1:How_Many))
   OPEN(FILE=File_Name,UNIT=1)
   DO I=1,How_Many
      READ (UNIT=1,FMT=*) Raw_Data(I)
   ENDDO

END SUBROUTINE Read_Data
```

```
SUBROUTINE Sort_Data(Raw_Data,How_Many)
IMPLICIT NONE
INTEGER , INTENT(IN) :: How_Many
REAL , INTENT(INOUT) , DIMENSION(:) :: Raw_Data

   CALL QuickSort(1,How_Many)

CONTAINS

   RECURSIVE SUBROUTINE QuickSort(L,R)
   IMPLICIT NONE
   INTEGER , INTENT(IN) :: L,R
   INTEGER :: I,J,tt
   REAL :: V,T

   i=l
   j=r
   v=raw_data( int((l+r)/2) )
   do
     do while (raw_data(i) < v )
          i=i+1
     enddo
     do while (v < raw_data(j) )
          j=j-1
     enddo
     if (i<=j) then
       t=raw_data(i)
       raw_data(i)=raw_data(j)
       raw_data(j)=t
       i=i+1
       j=j-1
     endif
     if (i>j) exit
   enddo

   if (l<j) then
     call quicksort(l,j)
   endif

   if (i<r) then
     call quicksort(i,r)
```

```
   endif

   END SUBROUTINE QuickSort

END SUBROUTINE Sort_Data

SUBROUTINE Print_Data(Raw_Data,How_Many)
IMPLICIT NONE
INTEGER , INTENT(IN) :: How_Many
REAL , INTENT(IN) , DIMENSION(:) :: Raw_Data
INTEGER :: I
   OPEN(FILE='SORTED.DAT',UNIT=2)
   DO I=1,How_Many
      WRITE(UNIT=2,FMT=*) Raw_Data(I)
   ENDDO
   CLOSE(2)
END SUBROUTINE Print_Data
```

We now have a choice of where we do the allocation. This is thus more flexible than having to do all allocation in the main program, which is effectively a more Fortran 77 style of programming.

28.2 Allocatable function result example

A function may return an array, and in this example the array allocation takes place in the function:

```
PROGRAM ch2802
IMPLICIT NONE

INTERFACE
   FUNCTION Running_Average(R,How_Many) RESULT(Rarray)
      IMPLICIT NONE
      INTEGER , INTENT(IN) :: How_Many
      REAL , ALLOCATABLE , DIMENSION (:) , &
         INTENT(IN) :: R
      REAL , ALLOCATABLE , DIMENSION(:) :: Rarray
   END FUNCTION Running_Average
END INTERFACE

INTERFACE
   SUBROUTINE Read_Data(File_Name,Raw_Data,How_Many)
      IMPLICIT NONE
```

```
      CHARACTER (LEN=*) , INTENT(IN) :: File_Name
      INTEGER , INTENT(IN) :: How_Many
      REAL , INTENT(OUT) , ALLOCATABLE , &
       DIMENSION(:) :: Raw_Data
   END SUBROUTINE Read_Data
END INTERFACE

INTEGER :: How_Many
CHARACTER (LEN=20) :: File_Name
REAL , ALLOCATABLE , DIMENSION(:)  :: Raw_Data
REAL , ALLOCATABLE , DIMENSION(:)  :: RA
INTEGER :: I
   PRINT * , ' How many data items are there?'
   READ  * , How_Many
   PRINT * , ' What is the file name?'
   READ '(A)',File_Name
   CALL Read_Data(File_Name,Raw_Data,How_Many)
   ALLOCATE(RA(1:How_Many))
   RA=Running_Average(Raw_Data,How_Many)
   DO I=1,How_Many
      PRINT *,Raw_Data(I),'    ' ,RA(I)
   END DO
END PROGRAM ch2802

FUNCTION Running_Average(R,How_Many) RESULT(Rarray)
INTEGER , INTENT(IN) :: How_Many
REAL , INTENT(IN) , ALLOCATABLE , DIMENSION(:) :: R
REAL , ALLOCATABLE , DIMENSION(:) :: Rarray
INTEGER :: I
REAL :: Sum=0.0
   ALLOCATE(Rarray(1:How_Many))
   DO I=1,How_Many
      Sum = Sum + R(I)
      Rarray(I)=Sum/I
   END DO
END FUNCTION Running_Average

SUBROUTINE Read_Data(File_Name,Raw_Data,How_Many)
IMPLICIT NONE
CHARACTER (LEN=*) , INTENT(IN) :: File_Name
INTEGER , INTENT(IN) :: How_Many
REAL , INTENT(OUT) , ALLOCATABLE , &
```

```
   DIMENSION(:) :: Raw_Data
INTEGER :: I
   ALLOCATE(Raw_Data(1:How_Many))
   OPEN(FILE=File_Name,UNIT=1)
   DO I=1,How_Many
      READ (UNIT=1,FMT=*) Raw_Data(I)
   ENDDO
END SUBROUTINE Read_Data
```

This is a much more Fortran 90 way of thinking.

28.3 Allocatable structure component example

This example illustrates the use of ragged arrays without the use of pointers:

```
PROGRAM ch2803
IMPLICIT NONE
TYPE Ragged
   REAL , DIMENSION(:) , ALLOCATABLE :: Ragged_row
END TYPE Ragged
INTEGER :: I
INTEGER , PARAMETER :: N=3
TYPE (Ragged) , DIMENSION(1:N) :: Lower_Diag
   DO I=1,N
      ALLOCATE(Lower_Diag(I)%Ragged_Row(1:I))
      PRINT *,' Type in the values for row ' , I
      READ *,Lower_Diag(I)%Ragged_Row(1:I)
   END DO
   DO I=1,N
      PRINT *,Lower_Diag(I)%Ragged_Row(1:I)
   END DO
END PROGRAM ch2803
```

28.4 Summary

These features provide us with a safer way of addressing certain types of problems that would previously have had to be tackled using pointers.

28.5 Problem

These features are not available in all compilers. Try each example out with your compiler to determine the degree of standard conformance.

29

Fortran 2003 and the Enhanced Module Facility

Aim

The aim of this chapter is to provide a brief coverage of some of the key features of Fortran 2003.

29 Fortran 2003 and the Enhanced Module Facility

This standard was published in 2004 and the language is called Fortran 2003. This is the classic out by one that the three previous versions of the language shared:

- Fortran 77 (1978)
- Fortran 90 (1991)
- Fortran 95 (1996)

Fortran 2008 is already in the pipeline!

The enhanced module facility is a separate development, and came after the publication of the 2003 standard.

29.1 Derived type enhancements

In Fortran 90/95 each of the intrinsic types has a kind parameter and character type has a length parameter. Fortran 2003 makes this functionality available to derived types.

29.2 Object oriented programming support

The language now offers:

- Type extension - one type can extend another.
- Polymorphism - the type of a variable can vary at run time.
- Dynamic type allocation.
- SELECT TYPE construct.
- Type-bound procedures.

Thus many problems based on abstract data typing and object oriented programming are now easily programmed in Fortran.

29.3 Data manipulation enhancements

Data manipulation enhacements include:

- Allocatable components.
- Deferred type parameters.
- VOLATILE attribute.
- Explicit type specification in array constructors.
- INTENT specification of pointer arguments.

- Specified lower bounds of pointer assignment and pointer rank remapping.
- Extended initialization expressions.
- MAX and MIN intrinsics for character type.
- Enhanced complex constants.

29.4 Input/output enhancements

I/O enhacements include:

- Asynchronous transfer operations — this allows a program to continue to execute while an input/output transfer occurs.
- Stream access — which allows access to a file without reference to any record structure.
- User specified transfer operations for derived types.
- User specified control of rounding during format conversions.
- The FLUSH statement.
- Named constants for preconnected units.
- Regularisation of input/output keywords.
- Access to input/output error messages.

Some of the above have been available in current compilers but not in a portable and standard fashion.

29.5 Interoperability with the C programming language

The intention here is to provide interoperability of:

- Types: this includes intrinsic types, derived types and pointers.
- Variables: both scalar and array.
- Procedures: this requires an explicit interface.

This is done via an intrinsic module called ISO_BINDING_C and the BIND and VALUE attributes.

C and Fortran interoperability has been possible for a long time with most compilers, but again not in a standard and portable fashion.

29.6 Procedure pointers

Procedure pointers permit ways of manipulating data (methods in object oriented programming or OOP terminology) to be associated with objects (dynamic binding in OOP terminology).

29.7 Scoping enhancements

There is now the ability to rename defined operators (which supports greater data abstraction) and control host association into interface bodies.

29.8 Support for IEC 60559 (IEEE 754) exceptions and arithmetic

This extends the ISO TR 15580 requirements. There is also a new IEEE 754 standard due to be published and it is envisaged that there will be support for this too.

29.9 Support for international usage: (ISO 10646)

Fortran 90 introduced the possibility of multibyte character sets, which provides a foundation for supporting ISO 10646 (2000). This is a standard for 4-byte characters, which is wide enough to support all of the world's languages.

A new intrinsic function has been introduced to provide the kind value for a specified character set:

- SELECTED_CHAR_KIND(NAME) returns the kind value as a default INTEGER.
- NAME is a scalar of type default character. If it has one of the values DEFAULT, ASCII, and ISO_10646, it specifies the corresponding character set.

The Fortran character set now includes both upper-case and lower-case letters and further printable ASCII characters have been added as special characters:

- ~ Tilde
- \ Backslash
- [Left square bracket
-] Right square bracket
- ` Grave accent
- ^ Circumflex accent
- { Left curly bracket

- } Right curly bracket
- | Vertical bar
- # Number sign
- @ Commercial at

There is also the choice of a decimal or a comma in numeric formatted input/output.

29.10 Enhanced integration with the host operating system

A new intrinsic module, ISO_FORTRAN_ENV, contains the following constants:

- INPUT_UNIT, OUTPUT_UNIT, and ERROR_UNIT are default integer scalars holding the unit identified by an asterisk in a READ statement, an asterisk in a WRITE statement, and used for the purpose of error reporting, respectively.
- IOSTAT_END and IOSTAT_EOR are default integer scalars holding the values that are assigned to the IOSTAT= variable if an end-of-file or end-of-record condition occurs, respectively.
- NUMERIC_STORAGE_SIZE, CHARACTER_STORAGE_SIZE, and FILE_STORAGE_SIZE are default integer scalars holding the sizes in bits of a numeric, character, and file storage unit, respectively.

Some of the above functionality can be found in existing compilers, but again not in a standard and therefore portable fashion.

29.11 The ASSOCIATE construct

This construct links named entities with expressions or variables during the execution of its block. Constructs may be nested.

29.12 Enhanced modules facility

The module facilities introduced in Fortran 90 had some drawbacks that were not apparent at the time. They are not a problem for small to medium scale program development but become a major issue with large code suites owing to the compilation cascade problem. What was needed was a mechanism to effectively decouple the interface from the implementation.

This is provided by this proposal where the concept of a submodule is introduced. The interface can be defined in the main module and the actual implementation can be done in submodules.

29.13 Summary

There are no compilers at this time that fully support the above. We hope this has whetted your appetite for what will be possible in the future with Fortran 2003 conformant compilers.

30

Parallel Programming

"Once upon a time, a very long time ago now, about last Friday, Winnie-the-Pooh lived in a forest all by himself under the name of Sanders."

("*What does 'under the name' mean" asked Christopher Robin, "It means he had the name over the door in gold letters and lived under it"...*)

A.A. Milne., *Winnie-the-Pooh*

Aim

The aims of this chapter is to introduce some of the options for parallel programming.

30 Parallel Programming

There are a number of options in this area and there is a brief coverage of some of them below.

30.1 MPI

MPI (message passing interface) is the standard for multicomputer and cluster message passing introduced by the Message Passing Interface Forum April 1994:

- http://www.mpi-forum.org/index.html

Visit:

- http://www.tc.cornell.edu/

at Cornell University for details of the above in practice.

30.2 Co–array Fortran

Co-array Fortran (previously known as F—) is a small extension to Fortran 95. Visit:

- http://www.co-array.org/

for more details.

The syntax is architecture independent and may be implemented on:

- Distributed memory machines.
- Shared memory machines.
- Clustered machines.

It is currently tabled for inclusion in the Fortran 2008 standard.

30.3 Openmp

To quote their home page '*The OpenMP Application Program Interface (API) supports multi-platform shared-memory parallel programming in C/C++ and Fortran on all architectures, including Unix platforms and Windows NT platforms. Jointly defined by a group of major computer hardware and software vendors, OpenMP is a portable, scalable model that gives shared-memory parallel programmers a simple and flexible interface for developing parallel applications for platforms ranging from the desktop to the supercomputer.*'

More information can be found at:

- http://www.openmp.org/

30.4 PVM

Parallel Virtual Machine consists of a library and a run-time environment which allow the distribution of a program over a network of (even heterogeneous) computers. Visit

- http://www.epm.ornl.gov/pvm/
- http://www.netlib.org/pvm3/

for more details.

30.5 HPF

To quote their home page

- http://www.crpc.rice.edu/HPFF/home.html

'The High Performance Fortran Forum (HPFF), a coalition of industry, academic and laboratory representatives, works to define a set of extensions to Fortran 90 known collectively as High Performance Fortran (HPF). HPF extensions provide access to high-performance architecture features while maintaining portability across platforms.'

They also provide details of:

- Surveys of HPF compilers and tools.
- Currently available commercial HPF compilers.
- Public domain HPF compilation systems.
- Research prototypes of HPF and HPF-related compilation systems.
- Mailing list.

30.6 Parallel programming and high-performance computing

Have a look at

- http://suparum.rz.uni-mannheim.de/docs/ind.html

for a lot of links to supercomputing centres and information on parallel computing in general.

For details of the US Accelerated Strategic Computing Initiative — ASCI — visit:

- http://www.sandia.gov/ASCI/
- http://www.lanl.gov/projects/asci/asci.html
- http://www.llnl.gov/asci/

The following are some useful UK sites:

- http://www.epsrc.ac.uk/hpc
- http://www.csar.cfs.ac.uk/

The following site lists the top 500 supercomputers in the world:

- http://www.netlib.org/benchmark/top500.html

To see what can be done with all this processing power visit:

- http://www.met-office.gov.uk/

30.6.1 Summary

Fortran is evolving and has come a long way since the 1950s. It is now capable of solving a wide range of problems.

A number of Fortran parallel dialects have emerged, but, it is important to realise that they are dialects and not part of the Fortran standard, and hence using them cannot guarantee portability.

Computers capable of supporting multiple processors are dropping in price and coming within the reach of most people. Developments in this area open up the possibilities of solving problems previously only possible on supercomputers.

31

Miscellaneous

"The time has come,' the Walrus said,
  'To talk of many things:
of shoes–and ships–and sealing wax–
  of cabbages – and kings–
And why the sea is boiling hot–
  And whether pigs have wings."

Lewis Carroll, *Through the Looking Glass and What Alice Found There.*

Aim

The aim of this chapter is to provide a summary of what has been covered and help put some of the material into context. In particular:

- Program development and software engineering.
- Programming style — programs should be easy to read.
- Programming style — programs should behave well.
- Data structures.
- Algorithms.
- Recursion, and when not to use it.
- Structured programming and the GOTO statement.
- Efficiency, the space time trade off.
- Simple debugging guidelines.
- Numerical software sources.

There is much to be learnt concerning the discipline of programming that does appear rather nonsensical at first.

31 Miscellaneous

By now it should be apparent that coding is only one small part of programming. However, a thorough knowledge of a programming language is a prerequisite for long term success.

Owing to its history, Fortran has a number of drawbacks in terms of its syntax and semantics. There are some features that are quite clumsy in comparison to other, more modern languages. However, there are also disadvantages in starting afresh each time, and this is highlighted by the Algol W, Pascal, Modula, Modula 2, (Modula 3), Oberon, Oberon 2 development. Moving from one language to its successor requires code changes that involve varying degrees of effort.

31.1 Program development and software engineering

When one first starts programming the phrase software engineering will often appear meaningless. The problems that one solves when learning a programming language are by necessity small and amenable to fairly rapid solution and hence don't require too much thought and serious planning. This means that many people will initially have a rather simplistic attitude and approach to programming in the real world.

Consider the following classification, from Fairley (1985), *Software Engineering Concepts*:

Classification	Number of programmers	Time scale	Lines of code
Trivial	1	1–4 weeks	500
Small	1	1–6 months	1K–5K
Medium	2–5	1–2 years	5K–50K
Large	5–20	2–3 years	50K–100K
Very large	100–1000	4–5 years	1M
Massive	2000–5000	5–10 years	1M–10M

The development of reliable and correct programs requires increasing degrees of planning and organisation as one moves from trivial, to small, to medium and beyond. It is worthwhile looking again at the earlier coverage of systems analysis and

design to see what stages we need to go through in the process of software engineering.

There are some practical considerations that can be applied regarding our use of a programming language, in this case Fortran 90.

31.1.1 Modules

Modules have a very important role to play in software engineering. Their addition to Fortran has made the language a much better vehicle for the construction of large-scale, reliable and easily maintainable programs. They enable us to adhere to the two guidelines of logical coherence and independence.

How big should a program unit be? The rather trite statement here is *small is beautiful*. Research has consistently shown that the time taken to test and debug a program unit grows exponentially with program size. Thus we have the following:

Program size	Testing and debugging time
1 unit	1 unit
2 units	4 units
3 units	8 units
4 units	32 units
etc.	

Experience also shows that most program units are between 60 and 120 lines of code. The reasons for this are to do with page size, rather than anything wonderfully technical. It is what we can fit onto one or two pages, i.e., what we can examine and understand easily. If we have to flip back and forth then we quickly lose track of what is happening.

31.1.2 Programming style — Programs should be easy to read

Programs have to be read and understood by both computer systems (the compiler) and humans. Your time is a very valuable resource. It therefore pays to develop a good programming style. Clarity, simplicity and consistency are of the essence:

- Meaningful names, not too long, not too short.
- Comments should clarify the meaning of the code.

- Indentation and formatting should be used to help structure the program and make it easier to read and understand; pretty print utilities may be available to help tidy up code.

The aim is not a Nobel prize for literature, but rather a style that adds rather than detracts from understanding the meaning of the program.

31.1.3 Programming style — Programs should behave well

Programs that behave badly will not be used, and most people reading this will know programs that they have stopped using precisely because they don't behave well. There are a number of things to consider here:

- Robustness, e.g., a compiler should not abort at the first error, but rather continue until some error limit is reached, preferably under user control.
- Input validation should be carried out, and the first criterion is legal input data. A second criteria is to allow correction of invalid data without forcing the user to retype everything. The phrase *'garbage in garbage out'* immediately springs to mind!
- Defensive programming — carry out tests before undertaking an operation. This will trap many common run-time errors, e.g., inappropriate argument to a function like the tangent of 90 degrees.
- Graceful degradation, e.g., ignore the one erroneous record in a file and carry on processing the rest of the file.
- Stick to the standard — as was stated earlier this pays off in the protection of the investment in people, in portability and a known reference point. If you have to use nonstandard features then learn fully what that entails. The *apparently* identical language extension in two compilers can quite legitimately produce completely different results. Let the buyer beware!

31.2 Data structures

Data structures have an enormous role to play in programming. An acquaintance with the wide range of available data structuring techniques is another skill that needs to be developed.

31.3 Algorithms

Algorithms have an important role to play in programming. The ability to choose the most appropriate algorithm for a particular problem is still another skill that needs to be developed.

31.4 Recursion

Recursion is a very powerful tool in problem solving. However, there are occasions when the overhead of recursion can be a problem. In this case it may be necessary to attempt to remove the recursion. There are a number of books that address this issue.

31.5 Structured programming and the GOTO statement

Consider the task of painting the floorboards in a room. Imagine getting a brush and a can of varnish and starting at the door. At some stage we end up in in the corner of the room and we have no way of leaving the room without walking over the recently painted boards. No problem: we GOTO the door.

Whilst the above may strike one as silly, the intention is to highlight the problems that can be created by inadequate preparation and planning.

As Knuth makes clear in *Structured Programming with GOTO Statements* that the real issue is structured programming, and structured programming is not the process of writing programs and then eliminating their GOTO statements. The comment by W.W. Peterson in his paper (regarding the teaching of PL/I, where he taught students to use the GOTO in exceptional circumstances) highlights this point: "*A disturbingly large percentage of the students ran into situations that require GOTOs, and sure enough, it was often because* **while** *didn't work well to their plan, but almost invariably because their plan was poorly thought out.*"

We have left the coverage of the GOTO statement until the last chapter to try and get people to think of solving problems without its use. The more astute reader may have already noticed that we have several examples throughout the notes that use an implied GOTO. These are the CYCLE and EXIT statements in loops. There is nothing wrong with using a GOTO providing its meaning is clear.

The syntax of the statement is

```
GOTO label
```

where label is a string of one to five decimal digits. Any statement in a Fortran program may have a label, e.g.,

```
GOTO 100
```

commonly used with a logical IF statement, e.g.,

```
IF (Error) GOTO 1000
```

31.6 Efficiency, space-time trade-off

Efficiency is important, but the first priority must always be program correctness. A good understanding of the capabilities of the language, combined with a reasonable breadth of knowledge in data structuring and algorithms, is a necessary precursor to concerns regarding efficiency.

There is a simple trade-off available with many problems: space versus time. This means that the program will require a large amount of memory to solve a problem, and this will be reflected in a time reduction. Memory cannot be infinite on any system, so there will be instances when a longer execution time has to be endured owing to insufficient physical memory.

Thus it will often be necessary to have only part of the data in memory. We will have to use disk to store the rest of the data we are processing. In situations like this we recommend that you use unformatted files. As we stated earlier they offer no loss of precision, and carry none of the overhead involved in formatting.

31.7 Program testing

Simplistically this means choosing a suite of data set inputs that test the following:

- One or more commonly occurring cases.
- Limiting cases.
- Pathological cases.

Just because it works on a small range of test data does not mean that there are no bugs.

31.8 Simple debugging techniques

The first choice is to switch on all error testing that can be provided by the compiler, and flag all nonstandard language features. This will trap the most common error, which is array indexing going beyond the declared bounds, for any array data type.

Use of interface blocks will trap another very common error, which is parameter mismatch between the calling and called routine.

The simplest debugging technique is the inclusion of print statements to clearly identify where the problem lies and the state of the variables of interest. There is no substitute for sitting down and working through a listing of the program with sample runs to try and determine where problems lie.

31.9 Software tools

There will be a range of tools available that aid in the program development process for the hardware and software platform that you use.

31.9.1 Cross referencing

Good compilers will offer cross reference compilation options. It is probable that stand alone tools in this area will eventually become available over the Internet.

31.9.2 Pretty print

It is likely that tools to aid in consistent program style will become available over the Internet in the near future. NAG for example offers a tool to pretty print Fortran 90 programs.

31.9.3 NAGWare f90 Tools

The following tools are currently available:

- **Polisher**: Pretty prints Fortran 90 code.
- **Declaration Standardiser**: Standardises declarations of variables and parameters.
- **Precision Standardiser**: Modifies software to use parameterised precision.
- **Name Changer**: Changes names.

Additional tools will be added with later releases.

31.10 Numerical software sources

This software exists in two main forms.

Firstly as coded algorithms, which can be obtained in a variety of source forms, which you as end user include in your own program and compile with your particular compiler. Some of these are verified; others are made available with no warranty!

Secondly as commercially precompiled libraries for a variety of compilers, operating systems and hardware platforms. These are subject to rigorous testing by the suppliers and very well documented.

ACM — TOMS **T**ransactions **o**n **M**athematical **S**oftware

They publish mathematical software as part of their collected algorithms of the ACM, available on magnetic tape and diskette. Further information is available on the World Wide Web, URL, http://www.acm.org

These sources are subject to validation and corrections, and improvements are published.

31.10.1 Numerical Algorithms Group

This is one of the two major commercial providers of numeric and statistical software. Their home page is:

- http://www.nag.co.uk/

31.10.2 Visual Numerics

Visual Numerics are the other major commercial provider of numeric and statistical software. Their home page is:

- http://www.vni.com/index.html

The following is the library home page:

- http://www.vni.com/products/imsl/index.html

31.10.3 Netlib

To quote their home page *"The Netlib repository contains freely available software, documents, and databases of interest to the numerical, scientific computing, and other communities. The repository is maintained by AT&T Bell Laboratories, the University of Tennessee and Oak Ridge National Laboratory, and by colleagues world-wide. The collection is replicated at several sites around the world, automatically synchronised, to provide reliable and network efficient service to the global community.*"

Home page is:

- http://www.netlib.org/

The software is free but you use it at your own risk, no support offered, and their motto is, *Anything free comes with no guarantee!*

31.11 Coda

Good luck!

31.12 Bibliography: All sources (bar one) taken from comp.software-eng.

31.12.1 Software engineering

The best place to start is on USENET news. One of the FAQs is a comprehensive post on reading material for software engineers, and it is maintained by profes-

sional software engineers. The current top five are in order below, the sixth is recommended reading.

Pfleeger S., *Software Engineering: The Production of Quality Software*, Macmillan, 1991.

Pressman R., *Software Engineering: A Practitioner's Approach*, McGraw Hill, 1987.

Sage A., Palmer J.D., *Software Systems Engineering*, Not known.

Ghezzi C., Jayazeri M., Mandrioli D., *Fundamentals of Software Engineering*, Prentice-Hall, 1991.

Berzins V., Luqi, *Software Engineering with Abstractions*, Addison-Wesley, 1991.

Brooks Frederick P. Jr, *The Mythical Man Month: Essays of Software Engineering*, Addison-Wesley, 1995.

31.12.2 Programming style

Anand N., *Clarify Function!*, ACM SigPLAN Notices, 23(6), 69–79, 1988.

Henry S., A Technique for Hiding Proprietary Details While Providing Sufficient Information for Researchers; or, do you Recognise this Well Known Algorithm?, *Journal of Systems and Software,* 8(1), 3–11.

Brooks R., Studying Programmer Behaviour Experimentally: The Problems of Proper Methodology, *Communications of the ACM*, 23(4), 207–213.

31.12.3 Software testing

Beizer Boris, *Software Testing Techniques*, Van Nostrand-Reinhold, 1990.

Hetzel William C., *The Complete Guide to Software Testing*, 2nd edition, QED Information Services Inc, 1988.

Software Research Inc., *Testing Techniques Newsletter*, Software Research Inc.

31.12.4 Fun

Martin Gardner, *Lewis Carroll: The Annotated Alice*, Penguin, 1999.

- Martin Gardner has been writing articles on mathematics as fun for twenty years. Lewis Carroll, née Charles Lutwidge Dodgson was a lecturer in mathematics at Christ Church College, Oxford.

A Glossary

actual argument

A value (variable, expression or procedure) passed from a calling program unit to a subprogram unit.

adjustable array

An explicit-shape array that is a dummy argument to a subprogram.

algorithm

Derived from the name of the 9^{th} century Persian mathematician Abu Ja'far Mohammed ibn Musa al-Kuwarizmi (father of Ja'far Mohammed, son of Moses, native of Kuwarizmi), corrupted through western culture as Al-Kuwarizmi. Now a sequence of computations.

allocatable array

An array that has the ALLOCATABLE attribute.

argument

Exists in two forms; actual argument, which is in the calling routine and is one of a variable, expression or procedure, and dummy argument, which is in the called routine.

argument association

The process of matching up an actual argument and dummy argument during program execution.

array

An array is a data structure where each scalar element has the same type and kind. An array may be up to rank 7. It may be referenced by element (via subscripts), by section or as a whole.

array constructor

A mechanism used to initialise or give values to a one-dimensional array. The RESHAPE function can then be used to handle rank 2 and above arrays.

array element

A scalar item of an array. An array element is picked out by a subscript.

array element ordering

The elements of an array, regardless of rank, form a linear sequence. The sequence is such that the subscripts along the first dimension vary most rapidly.

array section

A part of an array. The actual set depends on the subscripts.

ASCII

American Standard Code for Information Interchange. See Appendix C.

association

The means by which an entity can be referenced by different names in one scoping unit, or one or more names in multiple scoping units.

assumed-length dummy argument

A dummy argument that inherits the length attribute of the actual argument.

assumed-shape array

A dummy argument that inherits the shape of the associated argument.

assumed-size array

A dummy array whose size is inherited from the associated actual argument.

attribute

A property of a data type, and specified in a type declaration statement.

automatic array

This is an explicit-shape array that is a local variable in a subprogram unit.

bound

The bounds of an array are the upper and lower limits of the index in each dimension.

character constant

A constant that is a string of one or more printable ASCII characters, enclosed in apostrophes (') or quotation mark (").

character string

A sequence of one or more characters. These are contiguous.

collating sequence

The order in which a set of characters is sorted by default. The standard does not require that a processor provide the ASCII encoding, but does require intrinsic functions that convert between the processor encoding and the ASCII encoding.

compilation unit

One or more source files that are compiled to form one object file.

component

Part of a derived type definition.

concatenate

Join together two or more character items using the character concatenation operator //.

conformable

Two arrays are said to be conformable if they have the same shape.

constant

A constant is a data object whose value cannot be changed. There are two kinds in Fortran: one is obtained using the PARAMETER statement; the other is a literal constant in an expression; e.g., with the expression 4*ATAN(1) both 4 and 1 are literal constants. It may be a scalar or an array.

contiguous

Normally applied to items that are adjacent in memory, e.g., characters in a character variable.

data entity

A data object that has a specific type.

data object

A data object is a constant, variable or part of a constant or variable.

data type

For each data type there are the following: 0. a name 1. a set of values from a domain; 2. a set of valid operations upon these values; 3. a display method. There are five predefined data types in Fortran and these are integer, real, complex, character and logical.

For integers the values are drawn from the domain of integer numbers, the valid operations are addition, subtraction, multiplication, division and exponentiation, and they are displayed as a sequence of digits.

declaration

A declaration is a nonexecutable statement that specifies attributes of a program element, e.g., specifying the dimension of an array and the type of a variable.

default kind

The kind type parameter which is used for one of Fortran's base types (integer, real, complex, character or logical) if one is not specified.

deferred-shape array

An allocatable array or an array pointer. The bounds are specified with a colon, (:).

defined

For a data object having a valid value.

derived type

A data type that is user defined and not one of the five intrinsic types.

dimension

An array can be from one to seven dimensioned inclusive. Also called the rank.

dummy argument

A variable name that appears in the bracketed or parenthesised list following the procedure name. (e.g., function or subroutine name). Dummy arguments take on the actual values of the corresponding arguments in the calling routine.

elemental

An operation that applies independently to each element in an array.

entity

Rather vague term covering a constant, variable, program unit, etc.

exceptional values

Normally restricted to real numbers and typically one of nonnormalised numbers, infinity, not-a-number (NaN) values, etc.

explicit interface

A mechanism to make information available between the calling routine and the called routine. This information includes the names of the procedures, the dummy arguments, the attributes of the arguments, the attributes of functions, and the order of the arguments.

explicit-shape array

A named array that has its bounds specified in each dimension.

expression

An expression is a sequence of operands and operators that specifies a computation.

extent

The number of elements of one dimension of an array. Also called the size.

external subprogram

An external subprogram is one that is global to the whole program.

function

One of the two procedure mechanisms available in Fortran along with the subroutine. They effectively provide a way of invoking a computation by using the function name, and return a result. There is the concept of type and kind for the result.

function reference

A function is invoked by the use of its name in an expression.

function result

The result value(s) from invoking a function.

generic

Simplistically the ability of a procedure to accept arguments of more than type. This facility is taken for granted with the intrinsic procedures, and users can now create their own generic procedures.

global

An entity that is available throughout the executable program. A global entity has global scope. See also scope and local scope.

host association

The mechanism by which a module procedure, internal procedure or derived type definition accesses entities of the host.

implicit interface

A procedure interface whose properties are not known within the scope of the calling routine.

inquiry function

A function whose result depends on the properties of the argument.

interface block

A sequence of statements starting with an INTERFACE statement and ending with an END INTERFACE statement.

interface body

The sequence of statements in an interface block between either a FUNCTION or SUBROUTINE statement and the corresponding END statement.

internal procedure

A procedure that is contained within an internal subprogram. The program unit containing the internal procedure is called the host. The internal procedure is local to the host and inherits the host environment through host association.

intrinsic procedure

One of the standard supplied procedures.

kind

For each of the five Fortran types (integer, real, complex, logical and character) there is the concept of kind. For example for integers it is common to find 8-bit, 16-bit and 32-bit implementations. Each of these has an associated kind type.

For real and complex types this enables us to choose both the range and precision of the numbers we work with.

For characters we can choose between character sets, which is of considerable use for working with different languages.

kind type parameter

An integer value used to identify the kind of one of the five base types, see above.

language extension

Most compiler implementations will provide language extensions. These are NOT part of the standard, and make porting code suites between different hardware and software platforms difficult and sometimes impossible.

linker

A program that is normally the final stage in the process of going from Fortran source to executable.

local entity

An entity that is only available within the context of a subprogram.

main program

A program unit that contains a PROGRAM statement.

module

A program unit that contains specifications and definitions that other program units can access and use.

module procedure

A function or subroutine defined within a module

name

An entity with a program, e.g., constant, variable, function result, procedure, program unit, dummy argument.

name association

This provides access to the same entity (either data or a procedure) from different scoping units by the same or a different name.

nesting

The placing of one entity within another, e.g., one loop within another or one subprogram within another.

nonexecutable statement

A language statement that describes program attributes, but does not cause any action when the program is executed.

object file

File created after successful compilation. Used by the linker to generate an executable.

parameter

Term used to describe two completely different things. 1. a named constant — and hence the PARAMETER attribute. 2. more generally equivalent to argument.

pointer

A data object that has the POINTER attribute.

pointer association

The association of a part of memory to a pointer by means of a target.

precision

The number of significant digits in a real number.

procedure

A function or subroutine.

procedure interface

The statements that specify the name of a procedure, the characteristics of that procedure, the name of the dummy arguments, the attributes of the dummy arguments the generic identifier (optional) for the procedure.

program

A program is an entity that can be compiled and executed on its own. There must be at least a declaration block and execution block.

program unit

A main program or a subprogram. The subprogram can be a function, subroutine or module.

rank

The rank of an array is the number of dimensions.

recursion

A property of a function or subroutine, and it means that the function or subroutine references itself directly or indirectly.

reference

a data object reference is the appearance of a named entity in an executable statement requiring the value of the object.

relational expression

An expression containing one or more of the relational operators and operands of numeric or character type.

scalar

A single data object of any type. A scalar has a rank of zero.

scalar variable

A variable of scalar type.

scope and scoping unit

The part of a program in which a name has a defined meaning. The name may be a named constant, a variable, a function, a procedure, or dummy argument. The part of the program is one of a program unit or subprogram, a derived type definition or a procedure interface body. Scoping units cannot overlap, but one scoping unit

may be contained in another. In the latter case we have an example of host association.

shape

The rank and extents of an array.

shape conformance

Generally means that two or more arrays have the same rank and extent.

size

The total number of elements in an array — the product of the extents.

source file

A file known to the operating system that contains the Fortran statements.

statement

An instruction in a programming language, normally classified as executable and nonexecutable.

stride

The increment in a subscript triplet.

structure

Either a scalar data object of derived type or a composite entity containing one or more subcomponents.

subprogram

A user written or supplied function or subroutine.

subroutine

A user subprogram that is invoked with the CALL statement. It can return one value, many values or no value at all to the calling program through the arguments.

subscript

A scalar integer expression used to select an element of an array

subscript triplet

A subscript triplet is a set of three values representing the lower bound of the array section, the upper bound of the array section, and the increment (stride) between them.

substring

A contiguous set of characters in a string.

target

A named data object associated with a pointer.

transformational function

An intrinsic function that is not elemental or inquiry.

truncation

For real numbers the approximation obtained by chopping off the fractional part of the number and working with the integer part.

For character variables removing one or more characters from a string.

type declaration

One of the nonexecutable statements in Fortran, and one of INTEGER, REAL, COMPLEX, CHARACTER, LOGICAL or TYPE.

underflow

A condition where the result of an arithmetic expression is smaller than the minimum value in the range for that data type.

user defined type

A data type that is defined by the user and not one of the intrinsic types.

variable

A data object that has an associated memory location whose value can be changed during program execution. A variable may be a scalar or an array.

B Sample Program Examples

There is a coverage of the standard that applies, where appropriate. The more curious and inquisitive user may be interested in the information held at

- www.iso.ch

which is the International Standards Organisations world wide web page.

Ada: ISO/IEC 8652:1995

```
WITH TEXT_IO;USE TEXT_IO;
PROCEDURE Add IS
   X1   : FLOAT;
   X2   : FLOAT;
   Sum  : FLOAT:=0.0;
BEGIN
PACKAGE FLT_IO IS NEW FLOAT_IO(FLOAT);
USE FLT_IO;
   PUT(" Type in the two numbers");
   GET(X1);
   GET(X2);
   Sum:=X1 + X2;
   NEW_LINE(1);
   PUT(X1);
   PUT(" + ");
   PUT(X2);
   PUT(" = ");
   PUT(Sum);
END Add;
```

Algol: Was ISO 1538, but this has been withdrawn.

Algol 68: No standard, but the major definition is in the Revised Report.

Apl: ISO 8485:1989.

Basic: ISO/IEC 10279:1991, Full Standard; ISO 6373:1984, Minimal Conformance.

```
100 PRINT " Type in two numbers"
200 INPUT A, B
300 C = A + B
400 PRINT A, " + ", B, " = ", C
```

C: ISO/IEC 9899:1990

```
# include <stdio.h>
main()
{ float a,b,sum;
   printf(" Type in two numbers ");
   scanf("%f",&a);
   scanf("%f",&b);
   sum=a+b;
   printf("%f",a);
   printf(" + ");
   printf("%f",b);
   printf(" = ");
   printf("%f",sum);
   printf("\n"); }
```

C++: 1997–1998

```
#include <iostream.hxx>
#include <math.h>
int main()
{    float a,b,sum;
   sum=0.0;
   cout < " Type in two numbers   " ;
   cin > a > b ;
   sum =  a + b ;
   cout < a < " + " < b < " = " < sum < "\n" ;
   return (0); }
```

Cobol: ISO/IEC 1989:1985

Fortran 90: ISO/IEC 1539:1990

```
PROGRAM Example
IMPLICIT NONE
REAL :: A
REAL :: B
REAL :: Sum=0.0
   PRINT * , ' Type in two numbers'
   READ * , A,B
   Sum = A + B
   PRINT * , A ,' + ', B , ' = ', Sum
END PROGRAM Example
```

ICON: No standard.

Lisp

Logo: No standard.

Modula 2: ISO/IEC Draft 10514

```
MODULE Example;
   FROM InOut IMPORT Write,WriteLn,WriteString;
   FROM InOut IMPORT ReadReal,WriteReal;
   VAR
      A,B : REAL;
      Sum : REAL;
BEGIN
   Sum := 0.0;
   WriteString(" Type in two numbers");
   WriteLn;
   ReadReal(A);
   ReadReal(B);
   Sum := A + B;
   WriteReal(A,10);
   WriteString(" + ");
   WriteReal(B,10);
   WriteString(" = ");
   WriteReal(Sum,10);
   WriteLn;
END Example.
```

Oberon: No standard.

Pascal: Pascal — ISO 7185:1990; Extended Pascal — ISO/IEC 10206: 1991

```
PROGRAM Example(INPUT,OUTPUT);
VAR
   A : REAL;
   B : REAL;
   Sum : REAL;
BEGIN
   WRITELN(' Type in two numbers');
   READLN(A,B);
   Sum := A + B;
   WRITELN(A, ' + ' , B ,' = ' , Sum)
END.
```

Postscript:

Prolog: ISO/IEC Draft 13211-1

SQL: ISO 9075:1992(E)

Simula: No international standard, but a Swedish one does exist.

Smalltalk:

Snobol:

C ASCII Character Set

0	nul	32		64	@	96	'
1	soh	33	!	65	A	97	a
2	stx	34	“	66	B	98	b
3	etx	35	#	67	C	99	c
4	eot	36	$	68	D	100	d
5	enq	37	%	69	E	101	e
6	ack	38	&	70	F	102	f
7	bel	39	'	71	G	103	g
8	bs	40	(	72	H	104	h
9	ht	41	)	73	I	105	i
10	lf	42	*	74	J	106	j
11	vt	43	+	75	K	107	k
12	ff	44	,	76	L	108	l
13	cr	45	-	77	M	109	m
14	so	46	.	78	N	110	n
15	si	47	/	79	O	111	o
16	dle	48	0	80	P	112	p
17	dc1	49	1	81	Q	113	q
18	dc2	50	2	82	R	114	r
19	dc3	51	3	83	S	115	s
20	dc4	52	4	84	T	116	t
21	nak	53	5	85	U	117	u
22	syn	54	6	86	V	118	v
23	etb	55	7	87	W	119	w
24	can	56	8	88	X	120	x
25	em	57	9	89	Y	121	y
26	sub	58	:	90	Z	122	z
27	esc	59	;	91	[	123	{
28	fs	60	<	92	\	124	|
29	gs	61	=	93	]	125	}
30	rs	62	>	94	^	126	~
31	us	63	? 1	95	_	127	del

D Intrinsic Functions and Procedures

The following abbreviations and typographic conventions are used in this appendix.

Argument type and result type:

I	Integer
R	Real
C	Complex
N	Numeric (any of integer, real, complex)
L	Logical
P	Pointer
T	Target
DP	Double precision
Char	Character, length = 1.
S	Character

Class

E	Elemental function
I	Inquiry function
T	Transformational function
S	Subroutine

See Chapter 14 for more information on these classifications.

Arguments in italics

ALL(Mask,*Dim*)

are optional arguments, i.e., Dim may be omitted in the example above.

Double precision

Before Fortran 90 if you required real variables to have greater precision than the default real then the only option available was to declare them as double precision. With the introduction of kind types with Fortran 90 the use of double precision

declarations is not recommended, and instead real entities with a kind type offering more than the default precision should be used.

Kind optional argument

There are several functions that have an optional argument Kind, e.g., AINT(A,Kind). If Kind is absent the result is the same kind type as the first argument, in this case A. If Kind is present the result has the kind type specified by this argument.

Result type

When the result type is the same as the argument type then the result is not just the same type as the argument but also the same kind.

Miscellaneous rules

When the argument is Back it is of logical type.

When the argument is Count_Rate, Count_Max, Dim, Kind, Len, Order, N_Copies, Shape, Shift, Values it is of integer type.

When the argument is Mask it is of logical type.

When the argument is Target it is of pointer or target type.

ABS(A)

Yields the absolute value unless A is complex; see below.

Argument: A **Type:** N

Result: As argument **Class:** E

Note: If A is complex (x,y) then the functions returns $\sqrt{x^2 + y^2}$

Example: R1=ABS(A)

ACHAR(I)

Returns character in the ASCII character set.

Argument: I **Type:** I

Result: Char **Class:** E

Example: C=ACHAR(I)

ACOS(X)

Arccosine (inverse cosine).

Argument: X **Type:** R

Result: As argument **Class:** E

Note: $|x| \leq 1$

Example: Y=ACOS(X)

ADJUSTL(String)

Adjust string left, removing leading blanks and inserting trailing blanks.

Argument: String **Type:** S

Result: As argument **Class:** E

Example: S=ADJUSTL(S)

ADJUSTR(String)

Adjust string right, removing trailing blanks and inserting leading blanks.

Argument: String **Type:** S

Result: As argument **Class:** E

Example: S=ADJUSTR(S)

AIMAG(Z)

Imaginary part of complex argument.

Argument: Z **Type:** C

Result: As argument **Class:** E

Example: Y=AIMAG(Z)

AINT(A,*Kind*)

Truncation.

Argument: A **Type:** R

Result: As A **Class:** E

Argument: Kind **Type:** I

Example: Y=AINT(Z) and when Z=0.3 Y=0, when Z=2.73 Y=2.0, when Z=–2.73 Y=-2.0

ALL(Mask,*Dim*)

Determines whether all values are true in Mask along dimension Dim.

Argument: Mask **Type:** L

Result: L **Class:** T

Note: Dim must be a scalar in the range $1 \leq Dim \leq n$ where n is the rank of Mask. The result is scalar if Dim is absent or Mask has rank 1. Otherwise it works on the dimension Dim of Mask and the result is an array of rank n–1.

Example: T=ALL(M)

ALLOCATED(Array)

Returns true if array is allocated.

Argument: Array **Type:** Any

Result: L **Class:** I

Note: Array must be declared with the ALLOCATABLE attribute.

Example: IF (ALLOCATED(Array)) THEN ...

ANINT(A,*Kind)*

Rounds reals, i.e., returns nearest whole number.

Argument: A **Type:** R

Result: As A **Class:** E

Example: Z=ANINT(A), if A = 5.63 Z = 6, if A=-5.7 Z = -6.0

ANY(Mask,*Dim)*

Determines whether any value is true in Mask along dimension Dim.

Argument: Mask **Type:** L

Result: L **Class:** T

Note: Mask must be an array. The result is a scalar if Dim is absent or if Mask is of rank 1. Otherwise it works on the dimension Dim of Mask and the result is an array of rank n–1.

Example: T=ANY(A)

ASIN(X)

Arcsine.

Argument: X **Type:** R

Result: As argument **Class:** E

Example: Z=ASIN(X)

ASSOCIATED(Pointer,*Target)*

Returns the association status of the pointer.

Argument: Pointer **Type:** P

Result: L **Class:** I

Note:

1. If Target is absent then the result is true if POINTER is associated with a target, otherwise false.
2. If Target is present and is a target, the result is true if Pointer is currently associated with Target and false if it is not.
3. If Target is present and is a pointer, the result is true if both Pointer and Target are currently associated with the same target, and is false otherwise. If either Pointer or Target is disassociated the result is false.

Example: T=ASSOCIATED(P)

ATAN(X)

Arctangent.

Argument: X **Type:** R

Result: As argument **Class:** E

Example: Z=ATAN(X)

ATAN2(Y,X)

Arctangent of Y / X.

Argument: Y **Type:** R

Result: As arguments **Class:** E

Example: Z=ATAN2(Y,X)

BIT_SIZE(I)

Returns the number of bits, as defined by the numeric model for integer numbers in Chapter 8.

Argument: I **Type:** I

Result: As argument **Class:** I

Example: N_Bits=SIZE(I)

BTEST(I,Pos)

Returns true if the bit is set in the integer argument at the position given by the second argument.

Argument: I **Type:** I

Result: L **Class:** E

Example: T=BTEST(I,Pos)

CEILING(A,*Kind*)

Returns the smallest integer greater than or equal to the argument.

Argument: A **Type:** R

Result: I **Class:** E

Note:

If kind is present the result has the kind type parameter Kind.

Otherwise the result is of type default integer.

Example: I=CEILING(A) If A=12.21 then I=13, if A=-3.16 then I=-3

CHAR(I,*Kind*)

Returns the character in a given position in the processor collating sequence associated with the specified kind type parameter. Normally ASCII.

Argument: I **Type:** I

Result: CHAR **Class:** E

Example: C=CHAR(65) and for the ASCII character set C='A'.

CMPLX(X,*Y,Kind*)

Converts to complex from integer, real and complex.

Argument: X **Type:** N

Result: C **Class:** E

Note:
1. If X is complex and Y is absent it is as if Y were present with the value AIMAG(X).
2. If X is not complex and Y is absent, it is as if Y were present with the value 0.

Example: Z=CMPLX(X,Y)

CONJG(Z)

Conjugate of a complex argument.

Argument: Z **Type:** C

Result: As Z **Class:** E

Example: Z1=CONJG(Z)

COS(X)

Cosine.

Argument: X **Type:** R, C

Result: As argument **Class:** E

Note: The arguments of all trigonometric functions should be in radians, not degrees.

Example: A=COS(X)

COSH(X)

Hyperbolic cosine.

Argument: X **Type:** R

Result: As argument **Class:** E

Example: Z=COSH(X)

COUNT(Mask,*Dim*)

Returns the number of true elements in Mask along dimension Dim.

Argument: Mask **Type:** L

Result: I **Class:** T

Note: Dim must be a scalar in the range $1 \leq Dim \leq n$, where n is the rank of Mask. The result is scalar if Dim is absent or Mask has rank 1. Otherwise it works on the dimension Dim of Mask and the result is an array of rank n–1.

Example: N=COUNT(A)

CPU_TIME(Time)

Returns the processor time.

Argument: Time **Type:** R

Result: N/A **Class**: S

Example: CALL CPU_TIME(Time)

CSHIFT(Array,Shift,*Dim*)

Circular shift on a rank 1 array or rank 1 sections of higher-rank arrays.

Argument: Array	**Type:** Any
Result: As Array	**Class:** T

Note: Array must be an array, Shift must be a scalar if Array has rank 1, otherwise it is an array of rank n–1, where n is the rank of Array. Dim must be a scalar with a value in the range $1 \leq Dim \leq n$.

Example: Array=CSHIFT(Array,10)

DATE_AND_TIME(*Date,Time,Zone,Values*)

Returns the current date and time (compatible with ISO 8601:1988).

Argument: Date	**Type:** S
Result: N/A	**Class:** S

Time and Zone are of type S.

Note:
1. Date is optional and must be scalar and 8 characters long in order to return the complete value of the form CCYYMMDD, where CC is the century, YY is the year, MM is the month and DD is the day. It is INTENT(OUT).
2. Time is optional and must be scalar and 10 characters long in order to return the complete value of the form hhmmss.sss where hh is the hour, mm is the minutes and ss.sss is the seconds and milliseconds. It is INTENT(OUT).
3. Zone is optional and must be scalar and must be 5 characters long in order to return the complete value of the form hhmm where hh and mm are the time differences with respect to Coordinated Universal Time in hours and minutes. It is INTENT(OUT).
4. Values is optional and a rank 1 array of size 8. It is INTENT(OUT). The values returned are as follows:
Values(1) = the year
Values(2) = the month
Values(3) = the day
Values(4) = the time with respect to Coordinated Universal Time in minutes.
Values(5) = the hour (24 hour clock)
Values(6) = the minutes
Values(7) = the seconds
Values(8) = the milliseconds in the range 0–999.

Example: CALL DATE_TIME(D,T,Z,V)

DBLE(A)

Converts to double precision from integer, real, and complex

Argument: A **Type:** N

Result: DP **Class:** E

Example: D=DBLE(A)

DIGITS(X)

Returns the number of significant digits of the argument as defined in the numeric models for integer and reals in Chapter 8.

Argument: X **Type:** I,R

Result: I **Class:** I

Example: I=DIGITS(X)

DIM(X,Y)

Returns first argument minus minimum of the two arguments: X -MIN(X,Y).

Argument: X **Type:** I

Result: As arguments **Class:** E

Example: Z=DIM(X,Y)

DOT_PRODUCT(Vector_1,Vector_2)

Performs the mathematical dot product of two rank 1 arrays.

Argument: Vector_1 **Type:** Nt

Result: As arguments **Class:** T

Vector_2 is as Vector_1.

Note:
1. If Vector_1 is of type integer or real the result has the value SUM(Vector_1*Vector_2).
2. If Vector_1 is complex the result has the value SUM(CONJG(Vector_1)*Vector_2).
3. If Vector_1 is logical the result has the value ANY(Vector_1 .AND. Vector_2).

Example: A=DOT_PRODUCT(X,Y)

DPROD(X,Y)

Double precision product of two reals.

Argument: X **Type:** R

Result: DP **Class:** E

Example: D=DPROD(X,Y)

EOSHIFT(Array,Shift,*Boundary,Dim*)

End of shift of a rank 1 array or rank 1 section of a higher-rank array.

Argument: Array **Type:** Any

Result: As Array **Class:** T

Boundary is as Array.

Note: Array must be an array, Shift must be a scalar if Array has rank 1, otherwise it is an array of rank *n*–1, where *n* is the rank of Array. Boundary must be scalar if Array has rank 1, otherwise it must be either scalar or of rank *n*-1. Dim must be a scalar with a value in the range $1 \leq Dim \leq n$.

Example: A=EOSHIFT(A,Shift)

EPSILON(X)

Smallest difference between two reals of that kind. See Chapter 8 and real numeric model.

Argument: X **Type:** R

Result: As argument **Class:** I

Example: Tiny=EPSILON(X)

EXP(X)

Exponential, e^x.

Argument: X **Type:** R, C

Result: As argument **Class:** E

Example: Y=EXP(X)

EXPONENT(X)

Returns the exponent component of the argument. See Chapter 8 and the real numeric model.

Argument: X **Type:** R

Result: I **Class:** E

Example: I=EXPONENT(X)

FLOOR(A, *Kind)*.

Returns the greatest integer less than or equal to the argument

Argument: A **Type:** R

Result: I **Class:** E

Note:

If kind is present the result has the kind type parameter Kind, otherwise the result is of type default integer.

Example: I=FLOOR(A) and when A=5.2 I has the value 5, when A=-9.7 I has the value -10

FRACTION(X)

Returns the fractional part of the real numeric model of the argument See Chapter 8 and the real numeric model.

Argument: X **Type:** R

Result: As X **Class:** E

Example: F=FRACTION(X)

HUGE(X)

Returns the largest number for the kind type of the argument. See Chapter 8 and the real and integer numeric models.

Argument: X **Type:** I,R

Result: As argument **Class:** I

Example: H=HUGE(X)

IACHAR(C)

Returns the position of the character argument in the ASCII collating sequence.

Argument: C **Type:** Char

Result: I **Class:** E

Example: I=IACHAR('A') returns the value 65.

IAND(I,J)

Performs a logical AND on the arguments.

Argument: I **Type:** I

Result: As arguments **Class:** E

Example: K=IAND(I,J)

IBCLR(I,Pos)

Clears one bit of the argument to zero.

Argument: I **Type:** I

Result: As I **Class:** E

Note: $0 \le Pos < BIT_SIZE(I)$

Example: I=IBCLR(I,Pos)

IBITS(I,Pos,Len)

Returns a sequence of bits.

Argument: I **Type:** I

Result: As I **Class:** E

Note: $0 \le Pos$ and $(Pos + Len) \le BIT_SIZE(I)$ and $Len \ge 0$.

Example: Slice=IBITS(I,Pos,Len)

IBSET(I,Pos)

Sets one bit of the argument to one.

Argument: I **Type:** I

Result: As I **Class:** E

Note: $0 \le Pos < BIT_SIZE(I)$.

Example: I=IBSET(I,Pos)

ICHAR(C)

Returns the position of a character in the processor collating sequence associated with the kind type parameter of the argument. Normally the position in the ASCII collating sequence.

Argument: C **Type:** CHAR

Result: I **Class:** E

Example: I=ICHAR('A') would return the value 65 for the ASCII character set.

IEOR(I,J)

Performs an exclusive OR on the arguments.

Argument: I **Type:** I

Result: As I **Class:** E

Example: I=IEOR(I,J)

INDEX(String,Substring,*Back*)

Locates one substring in another, i.e., returns position of Substring in character expression String.

Argument: String **Type:** S

Result: I **Class:** E

Substring is of type S.

Note:
1. If Back is absent or present with the value .FALSE. then the function returns the start position of the first occurrence of the substring. If LEN(Substring) = 0 then one is returned.
2. If Back is present with the value .TRUE. then the function returns the start position of the last occurrence of the substring. If LEN(Substring) = 0 then the value (LEN(String) + 1) is returned.
3. If the substring is not found the result is zero.
4. If LEN(String) < LEN(Substring) the result is zero.

Example:
Where=INDEX(' Hello world Hello','Hello')
The result 2 is returned.
Where=INDEX(' Hello world Hello','Hello',.TRUE.)
The result 14 is returned.

INT(A,*Kind*)

Converts to integer from integer, real, and complex.

Argument: A **Type:** N

Result: I **Class:** E

Example: I=INT(F)

IOR(I,J)

Performs an inclusive OR on the arguments.

Argument: I **Type:** I

Result: As I **Class:** E

Example: I=IOR(I,J)

ISHFT(I,Shift)

Performs a logical shift. The bits of I are shifted by Shift positions.

Argument: I **Type:** I

Result: As I **Class:** E

Note: $|\ Shift\ | \le BIT_SIZE(\ I\ )$

Example: I=ISHIFT(I,Shift).

ISHFTC(I,Shift,*Size*)

Performs a circular shift of the rightmost bits. The Size rightmost bits of I are circularly shifted by Shift positions.

Argument: I **Type:** I

Result: I **Class:** E

Note:
$|\ Shift\ | \le Size$
$0 \le Size \le BIT_SIZE(I)$.
If Size is absent it is as if it were present with the value of BIT_SIZE(I).
If Shift is positive the shift is to the left.
If Shift is negative the shift is to the right.
If Shift is zero no shift is performed.

Example: I=ISHFTC(I,Shift,Size)

KIND(X)

Returns the KIND type parameter of the argument.

Argument: X **Type:** Any

Result: I **Class:** I

Example: I=KIND(X)

LBOUND(Array,*Dim*)

Returns the lower bounds for each dimension of the array argument or a specified lower bound.

Argument: Array **Type:** Any

Result: I **Class:** I

Note:
$1 \le Dim \le n$, where n is the rank of Array. The result is scalar if Dim is present oth-

erwise the result is an array of rank 1 and size *n*.
The result is scalar if Dim is present, otherwise a rank 1 array and size *n*.

Example: I=LBOUND(Array)

LEN(String)

Length of a character entity.

Argument: String **Type:** S

Result: I **Class:** I

Example: I=LEN(String)

LEN_TRIM(String)

Length of character argument less the number of trailing blanks.

Argument: String **Type:** S

Result: I **Class:** E

Example: I=LEN_TRIM(String)

LGE(String_1,String_2)

Lexically greater than or equal to and this is based on the ASCII collating sequence.

Argument: String_1 **Type:** S

Result: L **Class:** E

String_2 is of type S.

Example: L=LGE(S1,S2)

LGT(String_1,String_2)

Lexically greater than and this is based on the ASCII collating sequence.

Argument: String_1 **Type:** S

Result: L **Class:** E

Example: L=LGT(S1,S2)

LLE(String_1,String_2)

Lexically less than or equal to and this is based on the ASCII collating sequence.

Argument: String_1 **Type:** S

Result: L **Class:** E

String_2 is of type S.

Example: L=LLE(S1,S2)

LLT(String_1,String_2)

Lexically less than and this is based on the ASCII collating sequence.

Argument: String_1 **Type:** S

Result: L **Class:** E

Example: L=LLT(S1,S2)

LOG(X)

Natural logarithm, $\log_e x$.

Argument: X **Type:** R, C

Result: As argument **Class:** E

Example: Y=LOG(X)

LOG10(X)

Common logarithm, log10.

Argument: X **Type:** R

Result: As argument **Class:** E

Example: Y=LOG10(X)

LOGICAL(L,*Kind*)

Converts between different logical kind types, i.e., performs a type cast.

Argument: L **Type:** L

Result: L **Class:** E

Example: L=LOGICAL(K,Kind)

MATMUL(Matrix_1,Matrix_2)

Performs mathematical matrix multiplication of the array arguments.

Argument: Matrix_1 **Type:** N,L

Result: As arguments **Class:** T

Matrix_2 is as Matrix_1.

Note:
1. Matrix_1 and Matrix_2 must be arrays of rank 1 or 2. If Matrix_1 is of numeric

type so must Matrix_2.
2. If Matrix_1 has rank 1, Matrix_2 must have rank 2.
3. If Matrix_2 has rank 1, Matrix_1 must have rank 2.
4. The size of the first dimension of Matrix_2 must equal the size of the last dimension of Matrix_1.
5. If Matrix_1 has shape (*n,m*) and Matrix_2 has shape (*m,k*) the result has shape (n,k).
6. If Matrix_1 has shape (*m*) and Matrix_2 has shape (*m,k*) the result has shape (*k*).
7. If Matrix_1 has shape (*n,m*) and Matrix_2 has shape (*m*) the result has shape (*n*).

Example: R=MATMUL(M_1,M_2)

MAX(A1,A2,*A3,...***)**

Returns the largest value.

Argument: A1 **Type:** I,R

Result: As arguments **Class:** E

A2, A3,.. are as A1.

Example: A=MAX(A1,A2,A3,A4)

MAXEPONENT(X)

Returns the maximum exponent. See Chapter 8 and numeric models.

Argument: X **Type:** R

Result: I **Class:** I

Example: I=MAXEXPONENT(X)

MAXLOC(ARRAY,*Dim,Mask***)**

Determine the location of the first element of Array having the maximum value of the elements identified by Mask if present.

Argument: Array **Type:** I,R

Result: I **Class:** T

Note:
0. Normally in Fortran 95 if you omit an optional argument you must use keywords for the rest. This intrinsic breaks this rule and DIM can be omitted and it is not necessary to use a keyword with Mask.
1. Array must be an array.
2. Mask must be conformable with Array
3. The result is an array of rank 1 and of size equal to the rank of Array.

4. If Dim is present the result is an array of the rank of Array reduced by one and with the shape of Array without the dimension Dim.

Example:

A=(/5,6,7,8/)

I=MAXLOC(A)

is (4), which is the subscript of the location of the first occurrence of the maximum value in the rank 1 array.

If $A = \begin{pmatrix} 1 & 8 & 5 \\ 9 & 3 & 6 \\ 4 & 2 & 7 \end{pmatrix}$

I = MAXLOC(A,dim=1)

is (2,1,3) returning the position of the largest in each column.

I = MAXLOC(A,dim=2)

is (2,1,3) returning the position of the largest in each row.

MAXVAL(Array,*Dim,Mask***)**

Returns the maximum value of the elements of Array along dimension Dim corresponding to the true elements of Mask.

Argument: Array	**Type:** I,R
Result: As argument	**Class:** T

Note:
$1 \le Dim \le n$, where n is the rank of Array. The result is scalar if Dim is absent, or Array has rank 1. Otherwise the result is an array of rank n-1.
If Array has size zero then the result is the largest negative number supported by the processor for the corresponding type and kind of Array.

Example:

MAXVAL((/1,2,3/)) returns the value 3.

MAXVAL(C,MASK=C < 0.0) returns the maximum of the negative elements of C.

For $B = \begin{pmatrix} 1 & 3 & 5 \\ 2 & 4 & 6 \end{pmatrix}$

MAXVAL(B,DIM=1) returns (2,4,6)

MAXVAL(B,DIM=2) returns (5,6)

MERGE(True,False,Mask)

Chooses alternative values according to the value of a mask.

Argument: True **Type:** Any

Result: As True **Class:** E

Example: for

For $True = \begin{pmatrix} 2 & 6 & 10 \\ 4 & 8 & 12 \end{pmatrix}$, $False = \begin{pmatrix} 1 & 5 & 9 \\ 3 & 7 & 11 \end{pmatrix}$ and $Mask = \begin{pmatrix} T & F & T \\ F & T & F \end{pmatrix}$

The result is $\begin{pmatrix} 2 & 5 & 10 \\ 3 & 8 & 11 \end{pmatrix}$

MIN(A1,A2,*A3,...*)

Chooses the smallest value.

Argument: A1 **Type:** I, R

Result: As arguments **Class:** E

Example: Y=MIN(X1,X2,X3,X4,X5)

MINEXPONENT(X)

Returns the minimum exponent. See Chapter 8 and numeric models.

Argument: X **Type:** R

Result: I **Class:** I

Example: I=MINEXPONENT(X)

MINLOC(Array,*Dim,Mask)*

Determine the location of the first element of Array having the minimum value of the elements identified by Mask.

Argument: Array **Type:** I,R

Result: I **Class:** T

Note:
0. Normally in Fortran 95 if you omit an optional argument you must use keywords for the rest. This intrinsic breaks this rule and Dim can be omitted and it is not necessary to use a keyword with Mask.
1. Array must be an array.
2. Mask much be conformable with Array.
3. The result is an array of rank 1 and of size equal to the rank of Array.

4. If DIM is present the result is an array of the rank of Array reduced by one and with the shape of Array without the dimension DIM.

Example: I=MINLOC(Array)

In the above example if Array is a rank 2 array of shape (5,10) and the smallest value is in position (2,1) then the result is the rank 1 array I with shape (2) and I(1)=2 and I(2)=1.

See MAXLOC for further examples.

MINVAL(Array,*Dim,Mask)*

Returns the minimum value of the elements of Array along dimension Dim corresponding to the true elements of Mask.

Argument: Array	**Type:** I,R
Result: As Array	**Class:** T

Note:$1 \le Dim \le n$, where n is the rank of Array. The result is scalar if Dim is absent, or Array has rank 1. Otherwise the result is an array of rank n–1.
If Array has size zero then the result is the largest negative number supported by the processor for the corresponding type and kind of Array.

Example:

MINAL((/1,2,3/)) returns the value 1.

MINVAL(C,MASK=C > 0.0) returns the minimum of the positive elements of C.

For $B = \begin{pmatrix} 1 & 3 & 5 \\ 2 & 4 & 6 \end{pmatrix}$

MINVAL(B,DIM=1) returns (1,3,5).

MINVAL(B,DIM=2) returns (1,2).

MOD(A,B)

Returns the remainder when first argument divided by second.

Argument: A	**Type:** I, R
Result: As arguments	**Class:** E

Note: If B=0 the result is processor dependent. For B √ 0 the result is A - INT(A/B) * B.

Example: R=MOD(A,B)
If A=8 and B=5 then R=3
If A=-8 and B=5 then R=-3

If A=8 and B=-5 then R=3
If A=-8 and B=-5 then R=-3

MODULO(A,B)

Returns the modulo of the arguments.

Argument: A **Type:** I,R

Result: As A **Class:** E

Note:
1. If B=0 then the result is processor dependent.
2. Integer A
The result is R where A= Q * B + R and Q is integer
for B>0, $0 \le R < B$
for B < 0, $B < R \le 0$
3. Real A
The result is A - FLOOR(A/B) * B.

Example: R=MODULO(A,B)
If A=8 and B=5 then R=3
If A=-8 and B=5 then R=2
If A=8 and B=-5 then R=-2
If A=-8 and B=-5 then R=-3

MVBITS(From,F_Pos,Len,To,T_Pos)

Copies a sequence of bits from one data object to another.

Argument: From **Type:** I

Result: N/A **Class:** S

All arguments are of integer type.

Note:
From must be INTENT(IN).
F_Pos must be INTENT(IN), F_Pos ≥ 0, F_Pos+Len ≤ BIT_SIZE(From).
Len must be INTENT(IN), Len ≥ 0.
To must be INTENT(INOUT).
T_Pos must be INTENT(IN), T_Pos ≥ 0, T_Pos + Len ≤ BIT_SIZE(To).

Example: CALL MVBITS(F,FP,L,T,TP)

NEAREST(X,Next)

Returns the nearest different number. See Chapter 8 and the real numeric model.

Argument: X **Type:** R

Result: As X **Class:** E

Next is of type R.

Example: N=NEAREST(X,Next)

NINT(A,*Kind*)

Yields nearest integer.

Argument: A **Type:** RI

Result: I **Class:** E

Note:
1. A > 0, the result is INT(A+0.5).
2. A ≤ 0, the result is INT(A-0.5).

Example: I=NINT(X)

NOT(I)

Returns the logical complement of the argument.

Argument: I **Type:** I

Result: As I **Class:** E

Example: I=NOT(I)

NULL(*Mold)*

Returns a disassociated pointer.

Argument: Mold **Type:** P

Result: As argument **Class:** T

Note:

If the argument Mold is present the result is the same as Mold.

Otherwise it is determined by context.

Example: REAL , POINTER :: P=>NULL()

PACK(Array,Mask,*Vector*)

Packs an array into an array of rank 1, under the control of a mask.

Argument: Array **Type:** Any

Result: As Array **Class:** T

Note:
1. Array must be an array.
2. Mask be conformable with Array.
3. Vector must have rank 1 and have at least as many elements as there are TRUE elements in Mask.
4. If Mask is scalar with the value TRUE. Vector must have at least as many elements as there are in Array.
5. The result is an array of rank 1.
6. If Vector is present the result size is that of Vector.
7. If Vector is not present the result size is ***t*****,** the number of TRUE elements in Mask, unless Mask is scalar with a value TRUE in which case the result size is the size of Array.

Example: R=PACK(A,M)

PRECISION(X)

Returns the decimal precision of the argument. See Chapter 8 and numeric models.

Argument: X	**Type:** R, C
Result: I	**Class:** I

Example: I=PRECISION(X)

PRESENT(A)

Returns whether an optional argument is present.

Argument: A	**Type:** Any
Result: L	**Class:** I

Note: A must be an optional argument of the procedure in which the PRESENT function reference appears.

Example: IF (PRESENT(X)) THEN ...

PRODUCT(Array,*Dim,Mask***)**

The product of all of the elements of Array along the dimension Dim corresponding to the TRUE elements of Mask.

Argument: Array	**Type:** N
Result: As Array	**Class:** T

Note:
1. Array must be an array.
2. $1 \leq$ Dim $\leq$ n where n is the rank of Array.
3. Mask must be conformable with Array.

4. Result is scalar if Dim is absent, or Array has rank 1, otherwise the result is an array of rank n–1.

Example:
1. PRODUCT((/1,2,3/)) the result is 6.
2. PRODUCT(C,Mask=C > 0.0) forms the product of the positive elements of C.
3. If $B = \begin{pmatrix} 1 & 3 & 5 \\ 2 & 4 & 6 \end{pmatrix}$

PRODUCT(B,DIM=1) is (2,12,30) and
PRODUCT(B,DIM=2) is (15,48)

RADIX(X)

Returns the base of the numeric argument. See Chapter 8 and numeric models.

Argument: X	**Type:** I,R
Result: I	**Class:** I

Example: Base=RADIX(X)

RANDOM_NUMBER(X)

Returns one pseudorandom number or an array of pseudorandom numbers from the uniform distribution over the range $0 \le x < 1$

Argument: X	**Type:** R
Result: N/A	**Class:** S

Note: X is INTENT(OUT).

Example: CALL RANDOM_NUMBER(X)

RANDOM_SEED(*Size,Put,Get***)**

Restarts (seeds) or queries the pseudorandom generator used by RANDOM_NUMBER.

Argument: Size	**Type:** I
Result: N/A	**Class:** S

All arguments are of integer type.

Note:
1. Size is INTENT(OUT). It is set to the number N of integers that the processor uses to hold the value of the seed.
2. Put is INTENT(IN). It is an array of rank 1 and size ≥ N. It is used by the processor to set the seed value.

3. Get is INTENT(OUT). It is an array of rank 1 and size ≥ N. It is set by the processor to the current value of the seed.

Example: CALL RANDOM_SEED

RANGE(X)

Returns the decimal exponent range of the real argument. See Chapter 8 and the numeric model representing the argument.

Argument: X **Type:** N

Result: I **Class:** I

Example: I=RANGE(N)

REAL(A,*Kind*)

Converts to real from integer, real or complex.

Argument: A **Type:** N

Result: R **Class:** E

Example: X=REAL(A)

REPEAT(String,N_Copies)

Concatenates several copies of a string.

Argument: String **Type:** S

Result: S **Class:** T

Example: New_S=REPEAT(S,10)

RESHAPE(Source,Shape,*Pad,Order)*

Constructs an array of a specified shape from the elements of a given array.

Argument: Source **Type:** Any

Result: As Source **Class:** T

Note:
1. Source must be an array. If Pad is absent or of size zero the size of Source must be ≥ PRODUCT(Shape).
2. Shape must be a rank 1 array and 0 ≤ size < 8.
3. Pad must be an array.
4. Order must have the same shape as Shape and its value must be a permutation of (1,2,... ,*n*) where *n* is the size of Shape. If absent it is as if it were present with the value (1,2,...,*n*).
5. The result is an array of shape, Shape.

Example:

RESHAPE((/1,2,3,4,5,6/),(/2,3/)) has the value $\begin{pmatrix} 1 & 3 & 5 \\ 2 & 4 & 6 \end{pmatrix}$

RESHAPE((/1,2,3,4,5,6/) , (/2,4/) , (/0,0/) , (/2,1/)) has the value $\begin{pmatrix} 1 & 2 & 3 & 4 \\ 5 & 6 & 0 & 0 \end{pmatrix}$

RRSPACING(X)

Returns the reciprocal of the relative spacing of model numbers near the argument value. See Chapter 8 and the real numeric model.

Argument: X **Type:** R

Result: As X **Class:** E

Example: Z=RRSPACING(X)

SCALE(X,I)

Returns $X * b^I$ where b is the base in the model representation of *X*. See Chapter 8 and the real numeric model.

Argument: X **Type:** R

Result: As X **Class:** E

I is of integer type.

Example: Z=SCALE(X,I)

SCAN(String,Set,Back)

Scans a string for any one of the characters in a set of characters.

Argument: String **Type:** S

Result: I **Class:** E

Note:
1. The default is to scan from the left, and will only be from the right when Back is present and has the value TRUE.
2. Zero is returned if the scan fails.

Example: W=SCAN(String,Set)

SELECTED_INT_KIND(R)

Returns a value of the kind type parameter of an integer data type that represents all integer values n with $-10^R < n < 10^R$

Argument: R **Type:** I

Result: I **Class:** T

Note:
R must be scalar.
If a kind type parameter is not available then the value –1 is returned.

Example: I=SELECTED_INT_KIND(2)

SELECTED_REAL_KIND(*P,R*)

Returns a value of the kind type parameter of a real data type with decimal precision of at least *P* digits and a decimal exponent range of at least *R*.

Argument: P and R **Type:** I

Result: I **Class:** T

Note:
1. *P* and *R* must be scalar.
2. The value –1 is returned if the precision is not available, the value -2 if the exponent range is not available, and –3 if neither is available.

Example: I=SELECTED_REAL_KIND(P,R)

SET_EXPONENT(X,I)

Returns the model number whose fractional part is the fractional part of the model representation of X and whose exponent part is I.

Argument: X **Type:** R

Result: As X **Class:** E

I is of integer type.

Example: Exp_Part=SET_EXPONENT(X,I)

SHAPE(Source)

Returns the shape of the array argument or scalar.

Argument: Source **Type:** Any

Result: I **Class:** I

Note:
1. Source may be array valued or scalar. It must not be a pointer that is disassociated or an allocatable array that is not allocated. It must not be an assumed-size array.
2. The result is an array of rank 1 whose size is equal to the rank of Source.

Example: S=SHAPE(A(2:5,-1:1)) yields S=(4,3)

SIGN(A,B)

Absolute value of A times the sign of B.

Argument: A **Type:** I, R

Result: As A **Class:** E

Note:

In the special case where B is zero normally the result would have the value ABS(A), but if B is one of the real kind types and the processor is able to distinguish between plus zero and minus zero then the result is ABS(A) if B is plus zero and the result is –ABS(A) if B is minus zero.

B is as A.

Example: A=SIGN(A,B)

SIN(X)

Sine.

Argument: X **Type:** R, C

Result: As argument **Class:** E

Note: The argument is in radians.

Example: Z=SIN(X)

SINH(X)

Hyperbolic sine.

Argument: X **Type:** R

Result: As argument **Class:** E

Example: Z=SINH(X)

SIZE(Array,*Dim*)

Returns the extent of an array along a specified dimension or the total number of elements in an array.

Argument: Array **Type:** Any

Result: I **Class:** I

Note:
1. Array must be an array. It must not be a pointer that is disassociated or an allocatable array that is not allocated. If Array is an assumed-size array Dim must be present with a value less than the rank of Array.

2. Dim must be scalar and in the range $1 \leq \text{Dim} \leq n$ where n is the rank of Array.
3. Result is equal to the extent of dimension Dim of Array, or if Dim is absent, the total number of elements of Array.

Example: A=SIZE(Array)

SPACING(X)

Returns the absolute spacing of model numbers near the argument value. See Chapter 8 and the real numeric model.

Argument: X **Type:** R

Result: As X **Class:** E

Example: S=SPACING(X)

SPREAD(Source,Dim,N_Copies)

Creates an array with an additional dimension, replicating the values in the original array.

Argument: Source **Type:** Any

Result: As Source **Class:** T

Note:
1. Source may be array valued or scalar, with rank less than 7.
2. Dim must be scalar and in the range $1 \leq \text{Dim} \leq n+1$ where n is the rank of Source.
3. N_Copies must be scalar.
4. The result is an array of rank $n+1$.

Example:
If A is the array (2,3,4) then SPREAD(A,DIM=1,NCOPIES=3) then the result is the array $\begin{pmatrix} 2 & 3 & 4 \\ 2 & 3 & 4 \\ 2 & 3 & 4 \end{pmatrix}$

SQRT(X)

Square root.

Argument: X **Type:** R, C

Result: As argument **Class:** E

Example A=SQRT(B)

SUM(Array,*Dim,Mask***)**

Returns the sum of all elements of Array along the dimension Dim corresponding to the true elements of Mask.

Argument: Array **Type:** N

Result: As Array **Class:** T

Note:
1. Array must be an array.
2. $1 \le \text{Dim} \le n$ where n is the rank of Array.
3. Mask must be conformable with Array.
4. Result is scalar if Dim is absent, or Array has rank 1, otherwise the result is an array of rank n–1.

Example:
1. SUM((/1,2,3/)) the result is 6.
2. SUM(C,Mask=C > 0.0) forms the arithmetic sum of the positive elements of C.
3. If $B = \begin{pmatrix} 1 & 3 & 5 \\ 2 & 4 & 6 \end{pmatrix}$

SUM(B,Dim=1) is (3,7,11)
SUM(B,Dim=2) is (9,12)

SYSTEM_CLOCK(*Count,Count_Rate,Count_Max***)**

Returns integer data from a real time clock.

Argument: Count **Type:** I

Result: N/A **Class:** S

Note:
1. Count is INTENT(OUT) and is set to a processor dependent value based on the current value of the processor clock or to -HUGE(0) if there is no clock. $0 \le \text{Count} \le \text{Count_Max}$.
2. Count_Rate is INTENT(OUT) and it is set to the number of processor clock counts per second, or zero if there is no clock.
3. Count_max is INTENT(OUT) and is set to the maximum value that Count can have or to zero if there is no clock.

Example: CALL SYSTEM_CLOCK(C,R,M)

TAN(X)

Tangent.

Argument: X **Type:** R

Result: As argument **Class:** E

Note: X must be in radians.

Example: Y=TAN(X)

TANH(X)

Hyperbolic tangent.

Argument: X **Type:** R

Result: As argument **Class:** E

Example: Y=TANH(X)

TINY(X)

Returns the smallest positive number in the model representing numbers of the same type and kind type parameter as the argument.

Argument: X **Type:** R

Result: As X **Class:** I

Example: T=TINY(X)

TRANSFER(Source,Mold,*Size*)

Returns a result with a physical representation identical to that of Source, but interpreted with the type and type parameters of Mold.

Argument: Source **Type:** Any

Result: As Mold **Class:** T

Warning: A thorough understanding of the implementation specific internal representation of the data types involved is necessary for successful use of this function. Consult the documentation that accompanies the compiler that you work with before using this function.

TRANSPOSE(Matrix)

Transposes an array of rank 2.

Argument: Matrix **Type:** Any

Result: As argument **Class:** T

Note: Matrix must be of rank 2. If its shape is (*n,m*) then the resultant matrix has shape (*m,n*).

Example: For $A = \begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{pmatrix}$ TRANSPOSE(A) yields $\begin{pmatrix} 1 & 4 & 7 \\ 2 & 5 & 8 \\ 3 & 6 & 9 \end{pmatrix}$

TRIM(String)

Returns the argument with trailing blanks removed.

Argument: String **Type:** S

Result: As String **Class:** T

Note: String must be a scalar.

Example: T_S=TRIM(S)

UBOUND(Array,*Dim*)

Returns all the upper bounds of an array or a specified upper bound.

Argument: Array **Type:** Any

Result: I **Class:** I

Note:
$1 \le Dim \le n$, where n is the rank of Array. The result is scalar if Dim is present otherwise the result is an array of rank 1 and size n.
Result is a scalar if Dim is present otherwise is an array of rank 1, and size n.

Example: Z=UBOUND(A)

UNPACK(Vector,Mask,Field)

Unpacks an array of rank 1 into an array under the control of a mask.

Argument: Vector **Type:** Any

Result: As Vector **Class:** T

Note:
1. Vector must have rank 1. Its size must be at least t, where t is the number of true elements in Mask.
2. Mask must be array valued.
3. Field must be conformable with Mask. Result is an array with the same shape as Mask.

Example:

With $Vector = (1,2,3)$ and $Mask = \begin{pmatrix} F & T & F \\ T & F & F \\ F & F & T \end{pmatrix}$ and $Field = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

The result is $\begin{pmatrix} 1 & 2 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 3 \end{pmatrix}$

VERIFY(String,Set,*Back*)

Verify that a set of characters contains all the characters in a string by identifying the position of the first character in a string of characters that does not appear in a given set of characters.

Argument: String **Type:** S

Result: I **Class:** E

Note:
1. The default is to scan from the left, and will only be from the right when Back is present and has the value TRUE.
2. The value of the result is zero if each character in String is in Set, or if String has zero length.

Example: I=VERIFY(String,Set)

E English and Latin Texts

YET IF HE SHOULD GIVE UP WHAT HE HAS BEGUN, AND AGREE TO MAKE US OR OUR KINGDOM SUBJECT TO THE KING OF ENGLAND OR THE ENGLISH, WE SHOULD EXERT OURSELVES AT ONCE TO DRIVE HIM OUT AS OUR ENEMY AND A SUBVERTER OF HIS OWN RIGHTS AND OURS, AND MAKE SOME OTHER MAN WHO WAS ABLE TO DEFEND US OUR KING; FOR, AS LONG AS BUT A HUNDRED OF US REMAIN ALIVE, NEVER WILL WE ON ANY CONDITIONS BE BROUGHT UNDER ENGLISH RULE. IT IS IN TRUTH NOT FOR GLORY, NOR RICHES, NOR HONOURS THAT WE ARE FIGHTING, BUT FOR FREEDOM - FOR THAT ALONE, WHICH NO HONEST MAN GIVES UP BUT WITH LIFE ITSELF.

QUEM SI AB INCEPTIS DIESISTERET, REGI ANGLORUM AUT ANGLICIS NOS AUT REGNUM NOSTRUM VOLENS SUBICERE, TANQUAM INIMICUM NOSTRUM ET SUI NOSTRIQUE JURIS SUBUERSOREM STATIM EXPELLERE NITEREMUR ET ALIUM REGEM NOSTRUM QUI AD DEFENSIONEM NOSTRAM SUFFICERET FACEREMUS. QUIA QUANDIU CENTUM EX NOBIS VIUI REMANSERINT, NUCQUAM ANGLORUM DOMINIO ALIQUATENUS VOLUMUS SUBIUGARI. NON ENIM PROPTER GLORIAM, DIUICIAS AUT HONORES PUGNAMUS SET PROPTER LIBERATEM SOLUMMODO QUAM NEMO BONUS NISI SIMUL CUM VITA AMITTIT.

from *'The Declaration of Arbroath'* c.1320. The English translation is by Sir James Fergusson.

F Coded Text Extract

OH YABY NSFOUN, YAN DUBZY LZ DBUYLTUBFAJ BYYBOHNX GPDA FNUZNDYOLH YABY YAN SBF LZ B GOHTMN FULWOHDN DLWNUNX YAN GFBDN LZ BH NHYOUN DOYJ, BHX YAN SBF LZ YAN NSFOUN OYGNMZ BH NHYOUN FULWOHDN. OH YAN DLPUGN LZ YOSN, YANGN NKYNHGOWN SBFG VNUN ZLPHX GLSNALV VBHYOHT, BHX GL YAN DLMMNTN LZ DBUYLTUBFANUG NWLMWNX B SBF LZ YAN NSFOUN YABY VBG YAN GBSN GDBMN BG YAN NSFOUN BHX YABY DLOHDOXNX VOYA OY FLOHY ZLU FLOHY. MNGG BYYNHYOWN YL YAN GYPXJ LZ DBUYLTUBFAJ, GPDDNNXOHT TNHNUBYOLHG DBSN YL RPXTN B SBF LZ GPDA SBTHOYPXN DPSENUGLSN, BHX, HLY VOYALPY OUUNWNUNHDN, YANJ BEBHXLHNX OY YL YAN UOTLPUG LZ GPH BHX UBOH. OH YAN VNGYNUH XNGNUYG, YBYYNUNX ZUBTSNHYG LZ YAN SBF BUN GYOMM YL EN ZLPHX, GANMYNUOHT BH LDDBGOLHBM ENBGY LU ENTTBU; OH YAN VALMN HBYOLH, HL LYANU UNMOD OG MNZY LZ YAN XOGDOFMOHN LZ TNLTUBFAJ.

G Formal syntax

Statement ordering

FORMAT statements may appear anywhere between the USE statement and the CONTAINS statement.

The following table summarises the usage of the various statements within individual scoping units.

Kind of scoping unit	Main program	Module	External sub program	Module sub program	Internal sub program	Interface body
USE	Y	Y	Y	Y	Y	Y
FORMAT	Y	N	Y	Y	Y	N
Misc Dec [1]	Y	Y	Y	Y	Y	Y
Derived type definition	Y	Y	Y	Y	Y	Y
Interface block	Y	Y	Y	Y	Y	Y
Executable statement	Y	N	Y	Y	Y	N
CONTAINS	Y	Y	Y	Y	N	N

[1] Misc Dec (Miscellaneous declaration) are PARAMETER statements, IMPLICIT statements, type declaration statements and specification statements.

Syntax summary of some frequently used Fortran constructs

The following provides simple syntactical definitions of some of the more frequently used parts of Fortran 95.

Main program

```
PROGRAM [ program-name ]
   [ specification-construct ] ...
   [ executable-construct ] ...
   [CONTAINS
   [ internal procedure ] ... ]
END [ PROGRAM [ program-name ] ]
```

Subprogram

```
procedure heading
   [ specification-construct ] ...
   [ executable-construct ] ...
   [CONTAINS
   [ internal procedure ] ... ]
procedure ending
```

Module

```
MODULE name
   [ specification-construct ] ...
   [CONTAINS
   subprogram
   [ subprogram ] ... ]
END [ MODULE   [ module-name ]
```

Internal procedure

```
procedure heading
   [ specification construct ] ...
   [ executable construct ] ...
procedure ending
```

Procedure heading

```
[ RECURSIVE ] [ type specification ] FUNCTION
function-name &
   ( [ dummy argument list ] ) [ RESULT ( result name
) ]
[ RECURSIVE ] SUBROUTINE subroutine name &
   [ ( [ dummy argument list ] ) ]
```

Procedure ending

```
END [ FUNCTION [ function name ] ]
END [ SUBROUTINE [ subroutine name ] ]
```

Specification construct

```
derived type definition
interface block
specification statement
```

Derived type definition

```
TYPE [[ , access specification ] :: ] type name
   [ PRIVATE ]
   [ SEQUENCE ]
   [ type specification [[ , POINTER ] :: ] component
specification list ]
   ...
   END TYPE [ type name ]
```

Interface block

```
INTERFACE [ generic specification ]
    [ procedure heading
      [ specification construct ] ...
   procedure ending ] ...
   [ MODULE PROCEDURE module procedure name list ] ...
END INTERFACE
```

Specification statement

```
ALLOCATABLE [ :: ] allocatable array list
DIMENSION array dimension list
EXTERNAL external name list
FORMAT ( [ format specification list ] )
IMPLICIT implicit specification
INTENT ( intent specification ) :: dummy argument name
list
INTRINSIC intrinsic procedure name list
OPTIONAL [ :: ] optional object list
PARAMETER ( named constant definition list )
POINTER [ :: ] pointer name list
PUBLIC [ [ :: ] module entity name list ]
PRIVATE[ [ :: ] module entity name list ]
SAVE[ [ :: ] saved object list ]
TARGET [ :: ] target name list
USE module name [ , rename list ]
USE  module name , ONLY : [ access list ]
type specification [ [ , attribute specification ] ...
:: &
      object declaration list
```

Type specification

```
INTEGER [ ( [ KIND= ] kind parameter ) ]
REAL[ ( [ KIND= ] kind parameter ) ]
COMPLEX[ ( [ KIND= ] kind parameter ) ]
CHARACTER[ ( [ KIND= ] kind parameter ) ]
CHARACTER[ ( [ KIND= ] kind parameter ) ] &
   [ LEN= ] length parameter )
LOGICAL[ ( [ KIND= ] kind parameter ) ]
TYPE ( type name )
```

Attribute specification

```
ALLOCATABLE
DIMENSION ( array specification )
EXTERNAL
INTENT ( intent specification )
INTRINSIC
OPTIONAL
PARAMETER
POINTER
PRIVATE
PUBLIC
SAVE
TARGET
```

Executable construct

```
action statement
case construct
do construct
if construct
where construct
```

Action statement

```
ALLOCATE ( allocation list ) [ ,STAT= scalar integer
variable ] )
CALL subroutinename [ ( [ actual argument specification
list] ) ]
CLOSE ( close specification list )
CYCLE [ do construct name ]
DEALLOCATE( name list ) [ , STAT= scalar integer
variable ] )
ENDFILE external file unit
```

```
EXIT [ do construct name ]
GOTO label
IF ( scalar logical expression ) action statement
INQUIRE ( inquire specification list ) [ output item
list ]
NULLIFY ( pointer object list )
OPEN ( connect specification list )
PRINT format [ , output item list ]
READ (i/o control specification list ) [ input item
list ]
READ format [ , output item list ]
RETURN [ scalar integer expression ]
REWIND ( position specification list )
STOP [ access code ]
WHERE ( array logical expression ) array assignment
expression
WRITE ( i/o control specification list ) [ output item
list ]
pointer variable => target expression
variable = expression
```

H Compiler Options

In this appendix we look at what compiler options there are that can help us at both compile time and run time.

CVF

/check or /check:all

Equivalent to: /check:(arg_temp_created, bounds, flawed_pentium, format, power, output_conversion, overflow, underflow).

/debug

If you specify /debug:full, /debug, /Zi, or /Z7, the compiler produces symbol table information needed for full symbolic debugging of unoptimised code and global symbol information needed for linking. This is the default for a debug configuration in the visual development environment.

/exe[:file]

The /exe or /Fe option specifies the name of the executable program (EXE) or dynamic-link library (DLL) file being created. To request that a DLL be created instead of an executable program, specify the /dll option.

/fltconsistency

The /fltconsistency or /Op option enables improved floating point consistency on ia32 systems. floating point operations are not reordered and the result of each floating point operation is stored into the target variable rather than being kept in the floating point processor for use in a subsequent calculation. This option is ignored on ia64 systems

/fpe:0

The /fpe:level option controls floating point exception handling at run time for the main program. This includes whether exceptional floating point values are allowed and how precisely run time exceptions are reported. The /fpe:level option specifies how the compiler should handle the following floating point exceptions:

When floating point calculations result in a divide by zero, overflow, or invalid operation. When floating point calculations result in an underflow. When a denormalised number or other exceptional number (positive infinity, negative infinity, or a NaN) is present in an arithmetic expression

/list

The /list or /Fs option creates a listing of the source file with compile time information appended. To name the source listing file, specify file.

/map

/map[:file], /nomap, or /Fmfile The /map or /Fm option controls whether or not a link map is created. To name the map file, specify file.

/nooptimize

/show

The /show option specifies what information is included in a listing. In the visual development environment, specify the Source Listing Options in the Listing File Compiler Option Category.

/traceback

The /traceback option requests that the compiler generate extra information in the object file that allows the display of source file traceback information at run time when a severe error occurs.

/warn:all

The /warn option instructs the compiler to generate diagnostic messages for defined classes of additional checking that can be performed at compile time.

Intel

/check:all

Determines whether several run time conditions are checked.keyword: all, none, [no]arg_temp_created, [no]bounds, [no]format, [no]output_conversion

/debug:full

Determines the type of debugging information generated by the compiler in the object file. keyword: minimal, partial, full, none.

/exe:%1intel

/[no]fltconsistency

Determines whether improved floating point consistency is used.

/fpe:0

Specifies floating point exception handling at run time for the main program; n = 0, 1, or 3. 0 - floating underflow results in zero; all other floating point exceptions abort execution

/[no]map[:name]

Determines whether the compiler generates a link map (optionally, named name).

/[no]stand[:keyword]

Tells the compiler to issue warnings for nonstandard Fortran language elements. keyword: f90, f95, none.

/[no]traceback

Specifies whether the compiler should generate extra information in the object file that allows the display of source file traceback information at run time when a severe error occurs.

/warn:all

/map

Lahey

-chk

Specify -chk to generate a fatal run time error message when substring and array subscripts are out of range, when non common variables are accessed before they are initialised, when array expression shapes do not match, and when procedure arguments do not match in type, attributes, size, or shape.

-f95

Specify -f95 to generate warnings when the compiler encounters nonstandard Fortran 95 code.

-g

Specify -g to instruct the compiler to generate an expanded symbol table and other information for the debugger.

-info

Specify -info to display informational messages at compile time. Informational messages include such things as the level of loop unrolling performed, variables declared but never used, divisions changed to multiplication by reciprocal, etc.

-lst

Specify -lst to generate a listing file that contains the source program, compiler options, date and time of compilation, and any compiler diagnostics.

-OUT

Default: the name of the first object or source file.

-map

Default: create a map file with same name as output file

-trap diou

The -trap option specifies how each of four numeric data processor (NDP) exceptions will be handled at execution time of your program.

-trace

The -trace option causes a call traceback with procedure names and line numbers to be generated with run time error messages.

-warn

-fullwarn provides the maximum level of warning and informational messages.

-xref

Specify -xref to generate cross-reference information. This information is shown in the listing file in addition to the information that the -lst option would provide.

NAG

-C

ompile code with all possible run time checks. all array calls do none present pointer

-float-store

gnu C based systems. Do not store floating point variables in machines with floating point registers wider than 64 bits.

-gline

Include line number information in run time error messages.

-ieee=stop

Enables all IEEE arithmetic facilities except for nonstop arithmetic. Execution is terminated on floating overflow, divide by zero or invalid operand.

-o output

-strict95

Salford

/CHECKMATE

A synonym for /FULL_UNDEF. /FULL_UNDEF implies /UNDEF which in turn implies /CHECK.

/DEBUG

causes FTN95 to generate symbolic information and to activate the symbolic debugger when fatal errors occur. /DEBUG is included in both /CHECK and

/UNDEF, which are normally preferred. /DEBUG can be used on its own in order to allow the debugger to be used on "dirty" code, which intentionally violates some of the rules of Fortran.

/FULL_DEBUG

Outputs full debugging information including PARAMETERs

/FULL_UNDEF

Like /UNDEF but also INTENT(OUT) arguments are initialised as undefined on entry to a procedure (see /INHIBIT_CHECK to switch this off) and by default character variables are initialised as undefined. The reading of an undefined value precipitates an error condition.

/link

Generate executable.

/list

/map

Control the output of a listing file.

/xref

Generates a crossreference of all variables in a program and subprograms.

The use of the Win32 /UNDERFLOW option ensures that the first occurrence of underflow in an arithmetical computation is treated as a failure and is not ignored as would otherwise be the case. A large number of occurrences of underflow during execution can result in long execution times because of the way in which the underflow condition is treated. If an underflow is trapped, the message

ERROR: Floating point arithmetic underflow

is output and the interactive debugger is entered. If underflows occur during program execution and the /UNDERFLOW option is not used, a message is output at the end of the run specifying the number of underflows that have occurred.

Index

A

A edit descriptor 186, 244

ABS function 205, 206, 211, 542

Accuracy 86, 102, 426, 476, 478–479

ACHAR function 211, 250, 542

ACOS function 205, 211, 542

ActiveX 49-50

Actual argument 299, 310, 313, 315, 346, 367, 425, 427

Ada 2, 9, 43-44, 56-58, 60, 64, 536

Addition 78, 80, 126, 133-135, 137, 139, 141, 143, 145, 147, 149, 260, 517

Addition operator 80, 437

Adjustable array 310–311, 520

ADJUSTL function 211, 250, 543

ADJUSTR function 211, 250, 543

AIMAG function 211, 543

AINT function 211, 542, 543

Algol 60 16, 38-41, 470

Algol 68 2, 40-41, 56, 536

Algorithm 28, 33-34, 105, 108, 221–222, 268, 340, 369, 397, 470–471, 478, 488, 511, 514, 518–519

ALL function 211, 541, 543

ALLOCATABLE arrays 119, 133

ALLOCATABLE attribute 52, 120, 149, 310, 315, 361, 520, 544

ALLOCATABLE dummy array 493–494

ALLOCATE statement 121, 149, 270, 288, 292, 424

Alternate RETURN 367–368

ANINT function 211, 544

ANY function 211, 544

APL 2, 41, 60

Argument 210, 212, 295, 359, 370, 390, 392–393, 398, 447, 450–457, 541–573
- actual 299, 310, 313, 315, 346, 367, 425, 427, 520
- allocatable dummy array argument 493, 494
- array 206, 313, 316, 317, 319, 320, 367, 554, 556, 567
- assumed-length 315, 316, 521

assumed-shape 310, 313, 315, 316, 319, 320, 336, 367, 521
assumed-size 310, 367, 521, 567, 568
character 315
dummy 52, 220, 299, 310, 311, 313, 315–316, 336, 346, 367, 424–427, 442– 445, 520–523
keyword and optional 425, 427
PRESENT intrinsic function 210, 426–427, 563
rank 2 and higher array arguments 316

Arithmetic 5, 77–79, 81, 83, 85, 87, 89, 91, 93, 95, 97, 99, 101, 103, 105, 116, 366, 473–475, 477, 479, 481, 483, 485, 487–491

Arithmetic assignment statement 68, 70, 78, 102, 213, 271

Arithmetic IF 366

Array constructor 140, 148

Array element 134, 148

Array element ordering 133–134, 138,142, 148, 170, 438, 520

Array functions 211

Array section 138

Arrays 107–149
adjustable 310–311, 520
allocatable 51, 119, 133, 270, 310 321, 425, 494, 520
assumed-shape 310, 313, 315–316 319–320, 336, 367, 521
assumed-size 310, 367, 521
automatic 310,322,424–425
bounds 134, 149, 310–311, 313 315, 317, 321, 478, 503, 516, 521
constructor 52, 133, 136, 140–141 148, 502, 520
conformable 134–135, 147, 149, 522
deferred shape 149, 310, 321, 361, 424, 523
element 133, 135, 170, 206, 246 446, 520
explicit shape 310–311, 313, 316–317, 367, 520–521, 523
extent 13–135, 149, 310, 313 315, 367, 524
rank 134–135, 138, 140–146, 148, 149, 310, 313, 315–317 361, 367, 424, 438, 444, 470, 503 520, 523, 527
section 133, 138, 140, 144–145 148, 168–169, 189, 438, 494, 520–521, 528
shape 134,142,542,565
size 110, 114, 119–120, 133–134 149, 270, 310, 313, 424–425, 524 528
stride 144, 147, 494, 528
whole array manipulation 135

ASCII character set 5, 242, 542, 546, 552

ASIN function 205, 211, 544

ASSIGN and assigned GOTO statements 367

Assigned FORMAT statements 367

Assignment statement 68, 70, 78, 102, 104, 112, 213, 270–271

ASSOCIATED function 273

Assumed length dummy argument 315–316, 521

Assumed-shape arrays 310, 313, 315–316, 319–320, 336, 367, 521

Assumed-size 310, 367, 521

ATAN function 205, 211, 522, 545

ATAN2 function 205, 211, 256, 545

Attribute specification 579

Automatic arrays 310, 322, 424–425

B

Basic 2, 41, 59–60, 536

BIT_SIZE function 210, 545

Blanks 179–180, 185, 232

Blanks, nulls and zeros 185

Block IF statement 225–226, 237

BTEST function 98–101, 211, 546

C

C 2, 41–42, 49–50, 53, 56, 58–59

C++ 2,48–50,56,58,60,508,537

CALL statement 295, 299, 307, 528

CASE statement 223, 229–230, 367–368

CEILING function 51, 211, 546

CHAR function 211, 249–250, 546

Character argument 315

Character functions 247

Character I/O 241–252

Character operators 244

CHARACTER statement 66–67, 241–252

Character string 250

CLOSE statement 151, 163, 176, 188, 195

CMPLX function 211, 254–256, 546

Co-array Fortran 508

Cobol 2, 37–38, 40, 60, 537

Collating sequence 248

Comments 66, 70–71, 73

Common mistakes 162

Compilation unit 522

Compilers used 6–7

Complex 89, 253–256, 297, 302, 305, 478, 541

Computational functions 211

Concatenate 565

Conformable 134

CONJG function 211, 255, 547

CONTAINS statement 219, 304, 576

Continuation character & 71

Control Structures 223–225, 227, 229, 231, 233, 235, 237, 239

Converting from Fortran 77 366–367, 369, 371, 373, 375, 377, 379, 381, 383, 385, 387,389, 391, 393, 395, 397,399, 401, 403, 405, 407, 409

COS function 204–205, 211, 254, 424 547

COSH function 211, 547

COUNT function 211 547

CSHIFT function 211, 548

CYCLE and EXIT 234, 515

CYCLE statement 223, 234

D

Data description statements 65

Data processing statements 70

Data structures 511,514

Data type 3–4, 41, 46–47, 51–52, 63, 65, 69, 82, 92–93, 226, 242 244, 250, 254, 256, 264–268, 270, 288, 346–347, 362, 410, 412, 427–428, 441, 446, 470, 481, 516, 521–522

DATE_AND_TIME subroutine 211, 326, 328, 334, 337, 352, 355–356, 455–456, 458–459,495, 548

DBLE function 211, 549

DEALLOCATE statement 270, 326, 328, 428, 579

Debugging 260, 512–513, 516, 581–582, 585

Declaration 370, 398, 448, 517, 574

Decremented features 366

Default kind 102, 523

Deferred-shape arrays 149, 310, 321, 361, 424, 523

Deleted features 366

Derived type definition 578

DIGITS function 102, 210, 549

DIM function 146, 211, 549, 557–558

DIMENSION attribute 3, 110, 112, 115, 119, 126, 129
  additional form 126

Division 78, 230

DO construct 130

DO loop 100, 113, 116, 118–119, 127–128, 130,137, 140, 169, 201, 284, 313, 325

DO statement 113, 126, 128–129

DO WHILE construct 212–215, 217, 224, 232–233, 236, 238, 278, 281–283, 317, 408–409, 414,416

DOT_PRODUCT function 136 141, 207, 211, 549

DOUBLE PRECISION 367, 369–370, 377

DPROD function 211, 549

Dummy argument 299, 523
  assumed-length 315, 316, 521
  assumed-shape 310, 313, 315, 316, 319, 320, 336, 367, 521
  assumed-size 310, 367, 521, 567, 568
  character 315
  explicit shape array310–311, 313, 316–317, 367, 520–521, 523
  Dummy procedure argument 425

Dynamic data structures 412, 470+

E

E edit descriptor 162

Editors 19–20

Efficiency 511,516

Elemental 206–207, 218, 411–412, 443–445, 541

Elemental functions 206, 218

Elemental subroutine 411–412, 445

Elements of a programming language 64

ELSE block 215–216, 228

ELSE IF 223, 229, 237–238

ELSEWHERE block 147

END DO statement 201, 230, 234

END FUNCTION statement 212–213, 220

END PROGRAM statement 67, 71

END SELECT statement 230–231, 238

Entity 523

Entity oriented declaration 125–126

EOSHIFT function 211, 550

EPSILON function 94, 96, 210, 550

Errors when reading 192

Evaluation and testing 31

Exception handling 50, 477, 480, 488, 581–582

EXIT statement 223, 230, 234, 515

EXP function 205, 211, 235–236, 239, 470, 550

Explicit interface 356, 368, 503, 523

Explicit-shape array 310–310, 520–521, 523

EXPONENT function 210, 550

Exponentiation operator 78, 80

Expressions 135, 259

Extent 134

External 370, 387, 392–393, 398, 576

F

F edit descriptor 151, 155

File name 164, 179, 193, 198, 316

FILE= specifier 163–164, 173, 197

Files 195–202
  unformatted 174–176, 191, 199

Fixed fields on input 180

FLOOR function 51, 211, 551

FMT= specifier 163–165

FORALL statement and construct 51, 133, 147–148

FORM= specifier 175,191

FORMAT statement 150–193

Formatted data 199

Fortran character set 72, 242, 251, 504

FRACTION function 210, 551

Functions 94, 203–205, 207, 209, 211, 213, 215, 217, 219, 221, 370, 398, 450–451, 455, 458, 478, 541–573
  arguments 219
  array 211
  computational 211
  elemental 206, 218, 411–412, 443–444
  generic 205–206, 210
  inquiry 210, 524
  internal 218
  intrinsic 203–212, 541–573
  pure 51, 203, 2128, 442–443
  recursive 203, 214–215, 219
  transfer and conversion 210
  transformational 203, 206
  user defined 203–212

G

Gaussian elimination 341, 356–357

Generic 205, 411, 427

Generic functions 205

Generic procedures 411, 427

Global 378

Good programming guidelines 73

GOTO statement 224, 237, 240, 367, 511, 515

H

High Performance Fortran 51, 147, 509

Host association 53, 504, 524

HPF 7, 51, 147, 509

HUGE function 94, 96, 102, 210, 551

I

I edit descriptor 162,180

IACHAR function 211, 250, 551

IAND function 211, 551

IBCLR function 211, 552

IBITS function 211, 552

IBSET function 211, 552

ICHAR function 211, 249, 552

ICON 2, 46, 538

IEEE 5, 52–53, 57, 61, 94, 105, 473–477, 479–492, 504, 584

IEOR function 211, 552

IF statement 225–226, 228–229, 258, 366, 515

IMPLICIT NONE statement 66

Implied DO loops 168

INDEX function 247–248, 251

I/O 3–4, 12, 16, 66–67, 71, 122, 198, 200, 294, 337, 443, 503

INQUIRE statement 580

Inquiry functions 210

INT function 98

Integer data type 69, 71

Integer kind type 88–90

Intent 299

INTENT attribute 295, 299, 307, 443, 445

Interface 301, 304, 306, 336, 508, 576, 578

Interface block 301, 304, 306, 336, 576, 578

Internal functions 218

Internal procedure 577

Internal subroutine 325

Intrinsic functions 203–212, 541–573

IOR function 211, 553

ISHFT function 211, 554

ISHFTC function 211, 554

ISO TR 15580 472–492

ISO TR 15581 493–499

K

Keyword and optional argument 425, 427

Kind 88, 96–98, 542–544, 546, 551, 553, 556, 562, 565, 576

KIND function 90

Kind type parameter 90–91, 344, 361 523, 525

L

L edit descriptor 261

LaTeX 45

LBOUND function 210, 554

LEN function 210, 248, 250, 555

LEN_TRIM function 211, 248, 250, 555

LGE function 206, 211, 249–250, 555

LGT function 206, 211, 249–250, 555

Linked list 270

LINPACK 357,363

Lisp 2, 39–40, 56, 60, 538

LLE function 206, 211, 249–250, 555

LLT function 206, 211, 249–250, 556

Local variables 295, 298–300, 303, 306, 334–336, 359, 419, 443

Local variables and the SAVE attribute 295, 300

LOG function 205, 207–208, 211, 254 556

LOG10 function 205, 211, 556

Logical expression 223, 225

LOGICAL function 211, 556

Logical operators 257, 261

Logical variable 257

Logo 2, 44, 538

Lower bound 52, 144, 235, 315, 503, 554

M

Main program 296, 576

Maintenance 30, 32

Mantissa 92–93, 95, 101, 477, 479

Mask 146–148

Masked array assignment 146

MATMUL function 136, 211, 321–322 556

MAX function 52, 211, 503, 557

MAXEXPONENT function 210, 557

MAXLOC function 51, 211, 359, 361 557

MAXVAL function 211, 359, 361, 421 558

MERGE function 211, 559

MIN function 52, 211, 503, 559

MINEXPONENT function 210, 559

MINLOC function 51, 211, 559

MINVAL function 211, 560

MOD function 205, 208–212, 217, 220, 560

Modula 2 2, 29, 44, 47, 53, 58, 61, 268, 323, 471, 512, 538

Module 5, 51, 54–56, 301, 341–343, 345–347, 349, 351, 353, 355, 357, 359, 361, 363, 411, 501–503, 505, 513, 576–577
PUBLIC and PRIVATE attributes 446–448, 578–579
USE 342–344, 347, 368
USE ONLY 390–393, 395

Modules and packaging 411

Modules containing procedures 342, 349, 353

Modules for derived data types 346

Modules for global data 342

MODULO function 211, 561

MPI 508

Multiple statements 71

MVBITS function 211, 561

N

NEAREST function 210, 561

Nested user defined types 266

Nesting 122

Netlib 518

Networking 17

NINT function 211, 562

NOT function 211, 562

NULL function 51, 210, 275–276, 562

NULLIFY statement 270,279

O

Oberon 2 2, 46–47, 512

Object oriented programming 29, 48, 52, 502, 504

OPEN statement 163, 188, 193, 197

OPENMP 508

Operator and assignment overloading 411–412, 436

Operator hierarchy 259

Operators 78,80

Optional arguments 336, 425–427

Overflow 87, 153, 156–158, 473 477, 480, 581, 584

P

PACK function 211, 438–439, 562

Parameters 114,369,397

Pascal 2, 34, 41, 43–44, 56–57, 59–61, 222, 268, 470–471, 512, 538

PL/1 2,40

POINTER attribute 270–271, 526

Pointers 269–294
arrays of pointers 283
assignment statement 270–271
association status 270

Postscript 45, 56, 539

Precision 86, 96–98, 326, 330, 343–344, 357–359, 361–362, 418–419, 422, 424, 426, 517

PRECISION function 94, 96, 102, 210 563

PRESENT function 563

Pretty print 517

PRINT statement 67, 70–71, 152–153, 164, 177

PRIVATE attribute 446–448, 578–579

PRIVATE statement 578

PRODUCT function 211, 563

Program testing 516

Program unit 115, 148, 213–214, 299–300, 336, 342, 344–345 362, 425, 427, 441, 513, 527

Programming languages 2, 39, 65

Programming style 511, 513–514, 519

Prolog 2, 45, 56, 59, 370, 397, 539

PUBLIC attribute 446–448, 578–579

PUBLIC statement 578

PURE keyword 51, 203, 2128, 442–443

PVM 509

R

RADIX function 210, 564

RANDOM_NUMBER subroutine 211, 314, 564

RANDOM_SEED subroutine 211, 564

Range and precision of numbers 88, 90–91, 94, 525

RANGE function 210, 565

Rank 134–135, 138, 140–146, 148, 149, 310, 313, 315–317 361, 367, 424, 438, 444, 470, 503 520, 523, 52

Rank 2 and higher arrays as parameters 316

READ statement 67, 70, 187–188, 198, 200, 243, 279, 293, 367, 505
ADVANCE= 278–279, 293, 441
IOSTAT= 200–201, 278–279, 281, 283, 293, 505

Reading 179–181, 183, 185, 187, 189, 191, 193, 280

Reading in Data 179–181, 183, 185, 187, 189, 191, 193

REAL function 205, 211, 565

Real kind type 91, 94, 101, 221, 256, 568

Reals 155, 158, 181–182

Recursion 51, 214, 216–217, 222, 337, 511, 515

Recursive 214–216, 332, 337, 340

Recursive functions 214

Recursive subroutines 332

Referencing a subroutine 299

Relational expression 527

Relational operator 226, 527

REPEAT function 211, 250, 565

REPEAT UNTIL loop 232

Repetition 165–166

RESHAPE function 142, 148, 520

RETURN statement 219

REWIND 179, 188–189, 193–194, 580

Rounding and truncation 81

RRSPACING function 210, 566

S

SAVE attribute 295, 300

SCALE function 210, 488, 566

SCAN function 211, 250, 566

Scope 39, 295, 300

Scope of variables 295,300

Scoping unit 527

SELECT CASE statement 230–231, 238, 408–409

SELECTED_INT_KIND function 90

SELECTED_REAL_KIND function 90–92, 95, 210, 256, 567

SET_EXPONENT function 210, 567

Shape 134,142,542,565

SHAPE function 142,148,520

Shared DO termination and 366

SIGN function 51

Simula 2, 40, 46, 48, 56, 60, 417, 539

SIN function 204–207, 211, 254, 568

Singly linked list 278

SINH function 211, 568

SIZE function 210, 568

Skipping spaces and lines 187

Smalltalk 2, 47, 56, 58, 539

Snobol 2, 40, 46, 58, 60, 539

SPACING function 210, 569

Specification construct 577

Specification statement 578

SPREAD function 211, 569

SQL 2, 43, 45, 57, 539

SQRT function 205, 211, 219, 221, 228, 256, 569

Standardisation 42

Stepwise refinement 29

STOP statement 201

Stride 144, 147, 528

Structured programming 42,511,515

Subprogram 577

Subroutine 204, 295–297, 299–301, 303, 305, 307, 309– 311, 313, 315, 317, 319, 321, 323, 325, 327, 329, 331, 333, 335, 337, 339, 370, 387, 392–393, 398, 424, 439, 541
  actual arguments 299
  assumed-shape arrays 315, 320
  automatic arrays 310, 322
  contained 325–326
  dummy arguments 298–299, 313, 315–316, 336
  interface blocks 295, 301, 304, 306–307, 313, 336, 339
  internal 325
  INTENT attribute 295, 299, 307
  KEYWORD and optional arguments 425
  local variables and the SAVE attribute 295
  rank 2 and higher arrays as arguments 316

Substring 250,553

Subtraction operator 78

SUM function 207

Supplying your own functions 212

SYSTEM_CLOCK subroutine 211, 570

Systems Analysis and Design 33–34

T

TAN function 204–205, 211, 424, 570

TANH function 211, 571

Target 541–542, 545

Target attribute 270–271, 336

TeX 45, 59

TINY function 210, 571

Transfer and conversion functions 210

TRANSFER function 100, 211, 571

Transformational functions 206

TRANSPOSE function 211, 321–322, 571

Trees 440

TRIM function 211, 251, 572

Triplet 144, 147–148, 528

Truncation 82, 543

Type declaration 70–71

Type definition 264

U

UBOUND function 210, 572

Underflow 477, 480

Unformatted files 174, 176, 191, 199, 516

UNPACK function 211, 572

Upper bound 144, 235, 315, 572

USE 342–344, 347, 368, 576, 578

USE ONLY 390–393, 395, 578

User defined functions 296

User defined types 263–268

V

Variables 68–70, 114, 122–124, 128, 481, 503
status – undefined 70, 101, 270, 273

Vector 107, 110, 438, 549, 562–563, 572

VERIFY function 211, 251, 573

W

WHERE statement 133, 146–147

WHILE loop 232, 280

Whole array manipulation 135

WRITE statement 168, 170, 176, 188, 194–195, 505

Writing 36,164

X

X edit descriptor 160