



EPSRC

Introduction to Fortran 95



Reusing this material



This work is licensed under a Creative Commons Attribution-NonCommercial-ShareAlike 4.0 International License.

http://creativecommons.org/licenses/by-nc-sa/4.0/deed.en_US

This means you are free to copy and redistribute the material and adapt and build on the material under the following terms: You must give appropriate credit, provide a link to the license and indicate if changes were made. If you adapt or build on the material you must distribute your work under the same license as the original.

Note that this presentation contains images owned by others. Please seek their permission before reusing these images.



Acknowledgements

- A C Marshall from the University of Liverpool (funded by JISC/NTI) first presented this material. He acknowledged Steve Morgan and Lawrie Schonfelder.
- Helen Talbot and Neil Hamilton-Smith from the University of Edinburgh took the overheads from that course and worked on them to produce the associated Student Guide.
- Subsequent revisions of the material have been made by Kenton D'Mellow and Steve Thorn from the University of Edinburgh (ARCHER and ECDF teams).



Learning Outcomes

- On completion of this course students should be able to:
 - Understand and develop modularised Fortran programs.
 - (Compile and run Fortran programs on ARCHER.)



ARCHER Guest Accounts

- Guest account is only for the duration of the course
 - You can log in after hours between course days
- You must agree to the ARCHER terms and conditions:
 - <http://www.archer.ac.uk/about-archer/policies/tandc.php>



Outline Timetable

- **Day 1**

- 09:30 LECTURE: Fundamentals of Computer Programming
- 11:00 BREAK: Coffee
- 11:30 PRACTICAL: Hello world, formatting, simple input
- 12:30 BREAK: Lunch
- 13:30 LECTURE: Logical Operations and Control Constructs
- 14:30 PRACTICAL: Numeric manipulation
- 15:30 BREAK: Tea
- 16:00 LECTURE: Arrays
- 17:00 PRACTICAL: Arrays
- 17:30 CLOSE



Outline Timetable

- **Day 2**

- 09:30 PRACTICAL: Arrays (cont'd)
- 10:15 LECTURE: Procedures
- 11:15 BREAK: Coffee
- 11:45 PRACTICAL: Procedures
- 12:45 BREAK: Lunch
- 13:45 LECTURE: Modules and Derived Types
- 15:15 BREAK: Tea
- 15:45 PRACTICAL: Modules, Types, Portability
- 17:30 CLOSE





EPSRC

ARCHER Service

Overview and Introduction



ARCHER in a nutshell

- UK National Supercomputing Service
- Cray XC30 Hardware
 - Nodes based on 2×Intel Ivy Bridge 12-core processors
 - 64GB (or 128GB) memory per node
 - 3008 nodes in total (72162 cores)
 - Linked by Cray Aries interconnect (dragonfly topology)
- Cray Application Development Environment
 - Cray, Intel, GNU Compilers
 - Cray Parallel Libraries (MPI, SHMEM, PGAS)
 - DDT Debugger, Cray Performance Analysis Tools



Storage

- /home – NFS, not accessible on compute nodes
 - For source code and critical files
 - Backed up
 - > 200 TB total
- /work – Lustre, accessible on all nodes
 - High-performance parallel filesystem
 - Not backed-up
 - > 4PB total
- RDF – GPFS, not accessible on compute nodes
 - Long term data storage



Getting access to ARCHER

- Standard research grant
 - Request Technical Assessment using form on ARCHER website
 - Submit completed TA with notional cost in J-eS
 - Apply for time for maximum of 2 years
- ARCHER Resource Allocation Panel (RAP)
 - Request Technical Assessment using form on ARCHER website
 - Submit completed TA with RAP form
 - Application for computer time only
- Instant Access – Pump-Priming Time
 - Request Technical Assessment using form on ARCHER website
 - Submit completed TA with 2 page description of work
 - Office decision on application



ARCHER Partners

- EPSRC
 - Managing partner on behalf of RCUK
- Cray
 - Hardware provider
- EPCC
 - Service Provision (SP) – Systems, Helpdesk, Administration, Overall Management (also input from STFC Daresbury Laboratory)
 - Computational Science and Engineering (CSE) – In-depth support, training, embedded CSE (eCSE) funding calls
 - Hosting of hardware – datacentre, infrastructure, etc.



Introduction to Fortran 95



Fundamentals of Programming

- A computer must be given a set of unambiguous instructions (a program)
- Programming languages have a precise syntax. They can be:
 - high-level, like Fortran, C or Java
 - low-level, like assembler code
- A compiler translates high-level to low-level



Fortran

- Fortran comes from FORmula TRANslation
- Defined by an international standard
- Each update removes obsolescent features, corrects any mistakes, adds a few new features.



Character Set

- Alphanumeric:
 - a-z, A-Z, 0-9, underscore
 - lower case letters are equivalent to upper case letters
- 21 symbols, shown in the table on page 6



Tab

- Tab character is not in the Fortran character set
- Using a Tab generates a warning message from the compiler



Intrinsic Data Types

- Two intrinsic type classes:
 - Numeric, for numerical calculations
 - integer
 - real
 - complex
 - Non-numeric, for text-processing and control
 - character
 - logical



Numeric Data Types

- Integer: stored exactly, often in the range $[-2147483648, 2147483647]$
- Real: stored as exactly as possible in the form of mantissa and exponent, *eg* 0.271828×10^1
- The range of the exponent is typically in $[-307, 308]$
- Complex: an ordered pair of real values



Integer literal constants

- An entity with a fixed value within some range

-333

-1

0

2

32767



Real literal constants

- An entity with a fixed value within some range

-333.0

-1.0

0.

2.0

32767.0

3.2767E+04



Non-numeric Data Types

- Character: for text-processing
- Logical: truth values for control



Character literal constants

- An entity with a fixed value

`"a"`

`"abc"`

`"abc and def"`

`"Isn't"`

`'Isn''t'`



Logical literal constants

- One of the two fixed values
 - .TRUE.
 - .FALSE.



Names

- Names may be assigned to programs, subprograms, memory locations (variables), labels
- Naming convention – names:
 - must be unique within programs
 - must start with a letter
 - may use letters, digits, and underscore
 - may not be longer than 31 characters



Spaces

- Spaces must not appear:
 - within keywords
 - within names
- Spaces must appear:
 - between keywords
 - between keywords and names



Implicit Typing

- An undeclared variable has an implicit type:
 - If 1st letter of name is in the range I to N then it is of type `INTEGER`
 - Otherwise it is of type `REAL`
- This is a terrible idea! Always use:

`IMPLICIT NONE`

which requires every variable to be declared.



Variable and value

- The formal syntax of a declaration of a variable of a given type is

```
<type> [, attribute-list] :: &  
    <variable-list> [=value]
```

```
INTEGER :: k = 4
```

```
REAL, PARAMETER :: pi = 3.14159
```



Numeric type declarations

INTEGER :: i, j

REAL :: p

COMPLEX :: cx



Non-numeric type declarations

```
LOGICAL      :: l1
```

```
CHARACTER   :: s
```

```
CHARACTER(LEN=12) :: st
```



Initial values

- Declaring a variable does not assign a value to it: until a value has been assigned the variable is known as an unassigned variable.

```
INTEGER  :: i=1, j=2
```

```
REAL     :: p=3.0
```

```
COMPLEX  :: cx=(1.0, 1.732)
```



Initial values

```
LOGICAL :: on=.TRUE., off=.FALSE.
```

```
CHARACTER :: s='a'
```

```
CHARACTER(LEN=12) :: st='abcdef'
```

- `st` will be padded to the right with 6 blanks



Initial values

- The only intrinsic functions which may be used in initialisation expressions are:
 - RESHAPE
 - SELECTED_INT_KIND
 - SELECTED_REAL_KIND
 - KIND



Constant values

- The parameter attribute is used to set an unalterable value in a variable:

```
REAL, PARAMETER :: pi = 3.141592
```

```
REAL, PARAMETER :: radius = 3.5
```

```
REAL :: circum = 2.0 * pi * radius
```

- The variable `circum` does not inherit the attribute `PARAMETER`



Parameter attribute

- Scalar named constant of type character:

```
CHARACTER (LEN=*) , PARAMETER :: &  
    son='bart' , dad="Homer"
```

- This is equivalent to:

```
CHARACTER (LEN=4) , PARAMETER :: &  
    son='bart'
```

```
CHARACTER (LEN=5) , PARAMETER :: &  
    dad="Homer"
```



Comments

- An exclamation mark makes the rest of the line a comment:

```
! Assign value 1 to variable i
```

```
i = 1      ! i holds the value 1
```

```
! Character context differs:
```

```
st = "No comment!"
```



Continuation lines

- Continuation lines (max. 39) are marked with an ampersand:

```
CHARACTER (LEN=*) , PARAMETER :: &  
    son = 'bart'
```

- Breaking character strings is possible (but recommended only if necessary)

```
CHARACTER (LEN=4) :: son = 'ba&  
&rt'
```



Assignment

- All elements of this should be of the same type class (can mix numeric types)
- Each type class has its own set of operators

```
k = k + 1;      a = b - c
```

```
kinship = son//' son of '//dad
```

```
truth = p1.and.p2
```



Numeric operators

* * exponentiation: exponent a scalar

* multiplication / division

+ addition - subtraction

Shown in decreasing order of precedence. The leftmost of two operators of the same precedence applied first.



Character operators

```
CHARACTER(LEN=6) :: str1="abcdef"
```

```
CHARACTER(LEN=3) :: str2="xyz"
```

```
str1(1:1)    ! Substring "a"
```

```
str1//str2   ! Concatenation
```

```
! giving "abcdefxyz"
```



Operator precedence

- Operators have the precedence shown in descending order in the table on page 11
- Parentheses () may be used
- Operators of equal precedence are applied in left to right sequence



Mixed type Numeric expressions

- Calculations must be performed (internally) between objects of the same type. This is not a restriction for the programmer
- Precedence of types is:

COMPLEX

REAL

INTEGER

- Result always of higher type



Mixed type assignment

`<integer variable> = <real expression>`

The `<real expression>` is evaluated, truncated, assigned to an `<integer variable>`

`<real variable> = <integer expression>`

The `<integer expression>` is evaluated, promoted to type real, assigned to a `<real variable>`



Integer division

- Any remainder is discarded:

$$12 / 4 \rightarrow 3$$

$$12 / 5 \rightarrow 2$$

$$12 / 6 \rightarrow 2$$

$$12 / 7 \rightarrow 1$$



WRITE statement

```
WRITE (*, *) <output_list>
```

- Write the items of <output_list> to the default output device using default formatting

```
WRITE (*, *) "k =", k
```



READ statement

```
READ(*,*) <input_list>
```

- Read the items of `<input_list>` from the default input device using default formatting

```
READ(*,*) x, y
```



WRITE statement

```
WRITE (*, *) <output_list>
```

- Write the items of <output_list> to the default output device using default formatting

```
WRITE (*, *) "k =", k
```



WRITE statement

- `WRITE (unit=u, fmt=<format_specification>)`
`<output_list>`
- Write the items of `<output_list>` to the device identified as unit `u` using the `<format_specification>`

```
WRITE (unit=6, fmt="(A3, I4)") &  
    "k =", k
```



WRITE statement

- Each `WRITE` statement begins output on a new record
- The `WRITE` statement can transfer any object of intrinsic type to the standard output
- Be aware of the reserved unit numbers: 0, 5, 6
 - 0 Standard Error (error output)
 - 6 Standard output (screen or redirect)
 - 5 Standard input (keyboard or redirect)



Narrow field width

```
INTEGER :: i = 12345, j = -12345
```

```
WRITE(unit=6,fmt="(2I5)") i, j
```

```
12345*****
```



READ statement

```
READ(*,*) <input_list>
```

- Read the items of `<input_list>` from the default input device using default formatting

```
READ(*,*) x, y
```



READ statement

```
READ (unit=u, fmt=<format_specification>)  
<input_list>
```

- Read the items of `<input_list>` from the device identified as unit `u` using the `<format_specification>`

```
READ (unit=5, fmt="(I4, F5.1)") i, r
```



Prompting for input

```
WRITE (*, "(a)", ADVANCE="no") &  
    "prompt text"
```

- Note that here the format specification has optionally been given as a character literal constant



File handling

- File name has to be linked to a unit number:

```
OPEN(unit=u, file=file_name)
```

- For example:

```
OPEN(unit=10, file="result")  
WRITE(unit=10, fmt="(i4, f4.1)") &  
i, r
```



File handling

- A file may be disconnected by reference to its unit number:

```
CLOSE (unit=u)
```

- For example:

```
CLOSE (unit=10)
```



Formatting input and output

- Conversion between computer code for storing items and the characters on keyboard or screen
- An edit descriptor is needed for each item to be converted



Edit descriptor: integer

- I_w Integer value in a field w symbols wide, possibly including a negative sign

$I5$

- *bbbb1*
- -5600



Edit descriptor: floating point

- $F_w.d$ Floating point number, field width w with d digits after the decimal point

$F7.2$

- $bbb1.00$
- -273.18
- Decimal point is always present



Edit descriptor: exponential

- $E_w.d$ Exponential form, field width w with d digits after the decimal point

$E9.2$

- $b0.10E+01$
- $-0.27E+03$



Edit descriptor: logical

- L_w Logical value in field width w
- $L1$
- T
- $L2$
- bT



Edit descriptor: alphanumeric

- A_n Characters in field width n

"FOUR"

- A_3 FOU

- A_4 FOUR

- A_5 FOUR***b***

*b*FOUR

input

output



Edit descriptor: general

- $Gw.d$ General edit descriptor
- For real or complex: $Ew'.d'$ or $Fw'.d'$
 where $w' = w - 4$
- For integer: Iw
- For logical: Lw
- For character: Aw



Spaces and newlines

- \backslash denotes a single space
- $n\backslash$ denotes n spaces
- \backslash denotes a newline
- $\backslash\backslash$ denotes 2 newlines
- $n\backslash$ denotes n newlines



Format specification

- This is a comma separated list of edit descriptors contained in (parentheses)
- There must be an edit descriptor for each item in the input or output list

(A4, F4.1, 2X, A5, F4.1)



Repeat factors

- For a single edit descriptor:

$(I2, I2, I2) \rightarrow (3I2)$

- For a sequence of edit descriptors:

$(2X, A5, F4.1, 2X, A5, F4.1) \rightarrow (2(2x, A5, F4.1))$



Unequal counts

- Number of edit descriptors less than number of items in the list:

(3 I 2) I, J, K, L

I, J, K

1st record

L

2nd record



Unequal counts

- Number of edit descriptors more than number of items in the list:

(5I2) I, J, K, L

I, J, K, L

1 record only



Writing a program

The main steps are:

1. Specify the problem
2. Analyse the steps to a solution
3. Write Fortran code
4. Compile the program and run tests



Format of Fortran code

- The program source code is essentially free format with:
 - up to 132 characters per line
 - significant spaces
 - ! Comments
 - & continuation lines of a statement
 - ; separating statements on a line



Program structure

```
PROGRAM optional_name  
! Specification part  
! Execution part  
END PROGRAM optional_name
```



Specification part

- Declare type and name of variables

```
IMPLICIT NONE
```

```
INTEGER :: i
```

```
REAL :: p, q
```

```
COMPLEX :: x
```

```
CHARACTER :: c
```

```
CHARACTER(LEN=12) :: cc
```



Execution part

```
WRITE(6, "(A)") "text string"  
READ(*, *) variable_name
```



Errors

- Compile time
 - Mistyped variable name
 - Syntactic error in code
- Run time
 - Numeric value falls outside valid range
 - Logical error takes execution to wrong part of program, maybe using unassigned variables



Practical 1

- Try the questions on page 22



Relational operators

- $>$ greater than
- $>=$ greater than or equal
- $<=$ less than or equal
- $<$ less than
- \neq not equal to
- $==$ equal to
- Type logical result from numeric operands



Complex operands

- If either or both operands being compared are complex then the only operators allowed are:

== and /=



Logical operators

- `.NOT.` `.true.` if operand `.false.`
- `.AND.` `.true.` if both operands `.true.`
- `.OR.` `.true.` if at least one operand
`.true.`
- `.EQV.` `.true.` if both operands same
- `.NEQV.` `.true.` if both operands different



IF statement

```
IF (<logical-expression>) &  
    <executable-statement>
```

- Examples:

```
IF (x > y) a = 3
```

```
IF (I /= 0 .AND. J /=0) k=1/(i*j)
```

```
IF ((I /= 0) .AND. (J /=0)) & k=1/(i*j)
```



IF statement

- There is no shorthand for multiple tests on one variable
- Example: do J and K each hold the same value as I?
`IF (I == J .AND. I == K) ...`



Real-valued comparisons

```
REAL      :: a, b, tol=0.001
```

```
LOGICAL  :: same
```

```
! Assign values to a and b
```

```
IF (ABS(a-b) < tol) same=.TRUE.
```



IF...THEN construct

```
IF (i == 0) THEN  
! condition true  
    WRITE(*,*) "I is zero"  
! more statements could follow  
END IF
```



IF...THEN...ELSE construct

```
IF (i == 0) THEN
! condition true
    WRITE(*,*) "I is zero"
ELSE
! condition false
    WRITE(*,*) "I is not zero"
END IF
```



IF...THEN...ELSE IF construct

```
IF (I > 17) THEN
    Write(*,*) "I > 17"
ELSE IF (I == 17) THEN
    Write(*,*) "I is 17"
ELSE
    Write(*,*) "I < 17"
END IF
```



Nested, Named IF constructs

```
outa: IF (a == 0) THEN
  Write(*,*) "a is 0"
  inna: IF (b > 0) THEN
    Write(*,*) "a is 0 and b > 0"
  END IF inna
END IF outa
```



Procedure calls

- In the program on page 29 we have:
`SQRT (REAL (D)) ! D of type integer`
- `REAL` returns a type real value of its argument `D`
- `SQRT` needs a type real argument to return its square root



SELECT CASE construct

```
SELECT CASE (i)
  CASE (2, 3, 5, 7)
    Write(6, "A10") "i is prime"
  CASE (10:)
    Write(6, "(A10)") "i >= 10"
  CASE DEFAULT
    Write(6, "(A22)") &
      "I not prime and I < 10"
END SELECT
```



Select case components

- The case expression must be scalar and of type INTEGER, LOGICAL or CHARACTER
- The case selector must be of the same type as the case expression



Unbounded DO loop

```
i = 0  
DO  
  i = i + 1  
  Write(6, "(A4, I4)") "i is", i  
END DO
```



Conditional EXIT from loop

```
i = 0  
DO  
    i = i + 1  
    IF (i > 100) EXIT  
    Write(6, "(A4, I4)") "i is", i  
END DO  
! EXIT brings control to here
```



Conditional CYCLE in loop

```
i = 0
DO
  i = i + 1
  IF (i > 49 .AND. i < 60) CYCLE
  IF (i > 100) EXIT
  Write(6,"(A4,I4)") "i is ", i
END DO ! CYCLE brings control to here
! EXIT brings control to here
```



Named, Nested loops

```
outa: DO
  inna: DO
    IF (a > b) EXIT outa
    IF (a == b) CYCLE outa
    IF (c > d) EXIT inna
  END DO inna
END DO outa
```



Indexed DO loops

```
DO i = 1, 100, 1  
! i takes the values 1,2,3..100  
END DO
```

- Index variable *i* must be a named, scalar, integer variable
- *i* takes values from 1 to 100 in steps of 1
- *i* must not be explicitly modified in the loop
- Step is assumed to be 1 if omitted



Upper bound not met

```
DO I = 1, 30, 2
```

```
! I takes values 1, 3, ..., 27, 29
```

```
END DO
```



Index decremented

```
DO I = 30, 1, -2  
  ! I takes values 30, 28, ..., 4, 2  
END DO
```



Zero-trip loop

```
DO I = 30, 1, 2  
  ! Zero iterations, loop skipped  
END DO
```



Missing stride

```
DO I = 1, 30  
  ! I takes values 1, 2, ..., 29, 30  
END DO
```



DO construct index

```
DO I = 1, n
  IF (I == k) EXIT
END DO
```

- $n < 1$, zero trip, I given value 1
- $n > 1$ and $n \geq k$, I same value as k
- $n > 1$ and $n < k$, I has value $n+1$



Practical 2

- Try the questions on page 36
 - You will need the two files: `statsa` and `statsb`
 - <http://tinyurl.com/archerf95files>



Arrays

- An array is a collection of values of the same type
- Particular elements in an array are identified by subscripting



One-dimensional array

```
REAL, DIMENSION(1:15) :: X
```

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
---	---	---	---	---	---	---	---	---	----	----	----	----	----	----



Two-dimensional array

```
REAL, DIMENSION(1:5,1:3) :: Y, Z
```

1, 1	1, 2	1, 3
2, 1	2, 2	2, 3
3, 1	3, 2	3, 3
4, 1	4, 2	4, 3
5, 1	5, 2	5, 3



Two-dimensional array

```
REAL, DIMENSION (-4:0, 0:2) :: B
```

-4, 0	-4, 1	-4, 2
-3, 0	-3, 1	-3, 2
-2, 0	-2, 1	-2, 2
-1, 0	-1, 1	-1, 2
0, 0	0, 1	0, 2

Array terminology

- Rank: number of dimensions, max 7
- Bounds: lower and upper limits of indices (default lower bound is 1)
- Extent: number of elements in a dimension
- Size: total number of elements
- Shape: ordered sequence of all extents
- Conformable: arrays of the same shape



Array declarations

- Each named array needs a type and a dimension:

```
REAL, DIMENSION(15) :: x
```

```
REAL, DIMENSION(1:5,1:3) :: y,z
```

```
INTEGER, PARAMETER :: lda=5
```

```
LOGICAL, DIMENSION(1:lda) :: ld
```



Array element ordering

- Fortran does not specify how arrays should be located in memory
- In certain situations element ordering is in column major form, *ie* the first subscript changes fastest



Array element ordering

1	6	11
2	7	12
3	8	13
4	9	14
5	10	15

Array Sections

- Specified by subscript-triplets for each dimension:
- [`<bound1>`] : [`<bound2>`] : [`<stride>`]
- `<bound1>`, `<bound2>` and `<stride>`
- must each be scalar integer expressions



Array Sections

- `REAL, DIMENSION(1:15) :: A`
- `A(:)` whole array
- `A(m:)` elements `m` to 15 inclusive
- `A(:n)` elements 1 to `n` inclusive
- `A(m:n)` elements `m` to `n` inclusive
- `A(::2)` elements 1 to 15 in steps of 2
- `A(m:m)` 1 element section of rank 1



Array Sections

- Given
- `REAL, DIMENSION(1:6, 1:8) :: P`
- `P(1:3, 1:4)` is a simple 3x4 sub-array
- `P(1:6:2, 1:8:2)` takes elements from alternate rows and alternate columns and is also a 3x4 sub-array



P(1:3,1:4)

■	■	■	■				
■	■	■	■				
■	■	■	■				



P(1:6:2,1:8:2)

■		■		■		■	
■		■		■		■	
■		■		■		■	



$P(3,2:7)$ rank-one $P(3:3,2:7)$ rank-two

Array conformance

- Arrays or sub-arrays conform if they have the same shape
- Conforming arrays can be treated as a single variable in an expression:

`c = d`

`c = 1.0`



Conformance

$$C = D$$

valid



Non-Conformance

1,1		
		5,3

$$B = A$$

1						15
---	--	--	--	--	--	----

same size, different shape: invalid



Elements

$A(1) = 0.0$! set one element to zero

$B(0,0) = A(3) + C(5,1)$

! Set an element of B to

! the sum of two other elements



Whole array expressions

$a = 0.0$! scalar conforms to any shape

$b = c + d$! b, c, d must be conformable

$e = \sin(f) + \cos(g)$! and so must e, f, g



WHERE statement

```
WHERE (<logical-array-expr>) &  
      <array-variable> = <expr>
```

For example:

```
WHERE (P > 0.0) P = log(P)
```



WHERE construct

```
WHERE (<logical-array-expr>
      <array-assignments>
END WHERE
```

For example:

```
WHERE (P > 0.0)
      X = X + log(P)
      Y = Y - 1.0/P
END WHERE
```



COUNT function

```
COUNT (<logical-array-expr>)
```

For example:

```
nonnegP = COUNT (P > 0.0)
```



SUM function

SUM(<array>)

For example:

sumP = SUM(P)



MOD function

$\text{MOD}(A, N)$

Returns the remainder of A modulo N

For example:

$P = \text{MOD}(P, 2)$

replaces each element of P by the remainder when that element is divided by 2



Program `old_times` (page 46)

- Uses `where`, `sum`, `count` (and `mod`)
- Takes array sections `r1(1:n)` and `r2(1:n)`



MINVAL function

`MINVAL (<array>)`

Returns the minimum value of an element of `<array>`

For example:

`minP = MINVAL (P)`



MAXVAL function

`MAXVAL (<array>)`

Returns the maximum value of an element of `<array>`

For example:

`maxP = MAXVAL (P)`



MINLOC function

MINLOC (<array>)

Returns a rank-one integer array of size equal to rank of <array> with the subscripts of the element of <array> with minimum value. MINLOC assumes the declared lower bounds of <array> were 1



MINLOC function

```
REAL, DIMENSION(1:6,1:8) :: P
INTEGER, DIMENSION(1:2) :: PRC
! Assign values to P
PRC = MINLOC(P)
! PRC(1) returns row subscript
! PRC(2) returns column subscript
```



MAXLOC function

MAXLOC (<array>)

Returns a rank-one integer array of size equal to rank of <array> with the subscripts of the element of <array> with maximum value. MAXLOC assumes the declared lower bounds of <array> were 1



MAXLOC function

```
REAL, DIMENSION(1:6,1:8) :: P
INTEGER, DIMENSION(1:2) :: PRC
! Assign values to P
PRC = MAXLOC(P)
! PRC(1) returns row subscript
! PRC(2) returns column subscript
```



Program seek_extremes (p48)

- Uses `minval`, `maxval`, `minloc` and `maxloc` on the whole rank 2 array `magi`



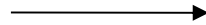
Array input/output

- Elements of an array of rank greater than 1 are stored in column major form
- For arrays of rank 2 the intrinsic function `TRANPOSE` changes rows and columns



TRANSPOSE function

1	4	7
2	5	8
3	6	9



1	2	3
4	5	6
7	8	9



Array constructors

Give arrays or array-sections specific values: arrays must be rank 1 and conform

```
INTEGER :: i
```

```
INTEGER, DIMENSION(1:8) :: ints
```

```
ints=(/100,1,2,3,4,5,6,100/)
```

```
ints=(/100,(i, i=1,6), 100/)
```



RESHAPE intrinsic function

- Form is `RESHAPE (<source>, <shape>)`

`INTEGER, DIMENSION(1:2,1:2) :: a`

`a=RESHAPE (/1,2,3,4/), (/2,2/))`

1	3
2	4



Named Array Constants

```
INTEGER, DIMENSION(3), &  
  PARAMETER :: Unit_vec = (/1,1,1/)
```

```
INTEGER, DIMENSION(3,3), &  
  PARAMETER :: Unit_matrix = &  
  RESHAPE(/1,0,0,0,1,0,0,0,1/), (/3,3/))
```



Allocatable array declaration

- Declare the array giving its type, rank, the attribute `allocatable`, and name:

```
REAL, DIMENSION(:), &  
    ALLOCATABLE :: ages
```



Allocatable array allocation

- Specify the bounds of the array and optionally check for success

```
ALLOCATE (ages (1:60), STAT=ierr)
```

- If the integer variable `ierr` returns 0 then the array `ages` has been allocated



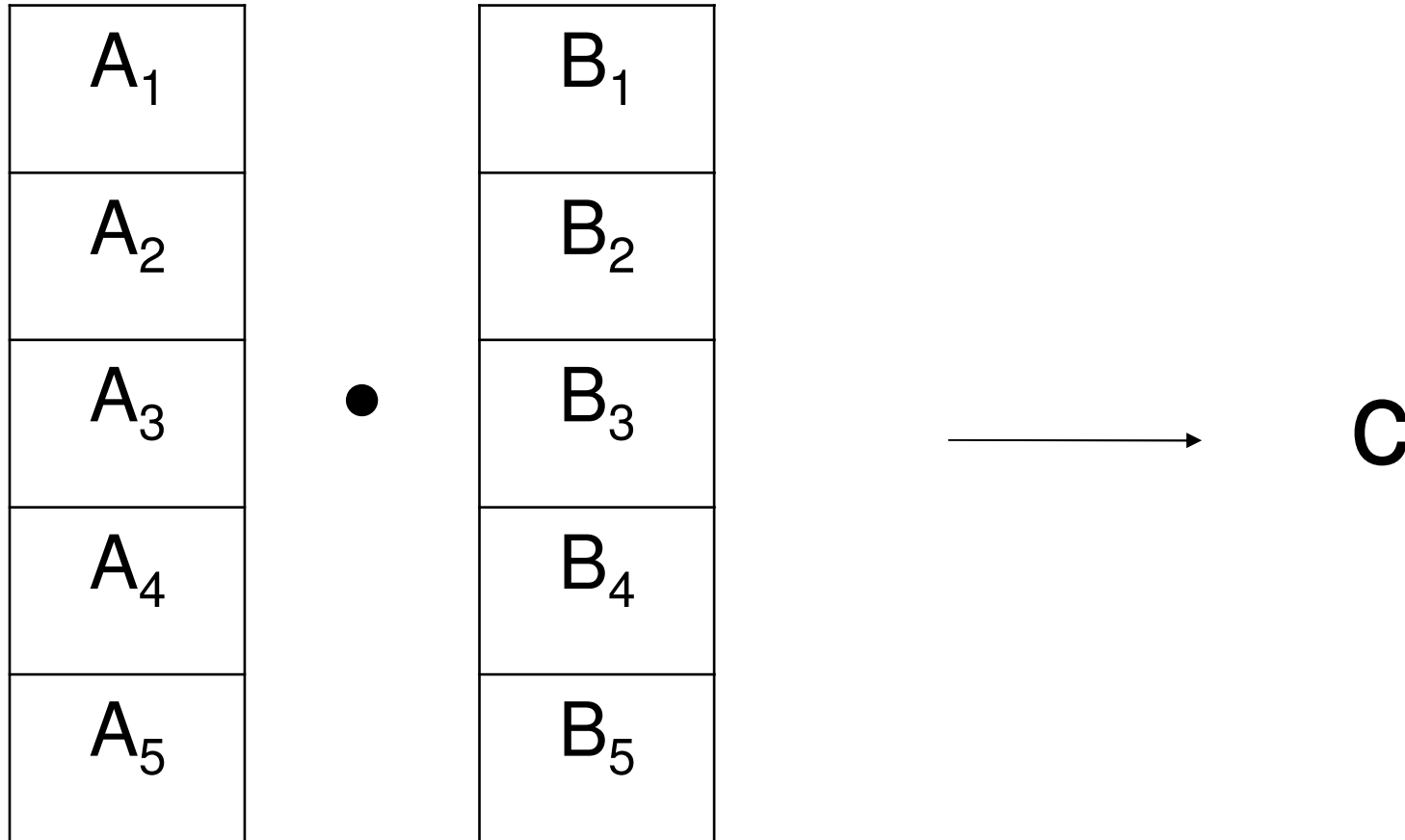
Deallocating arrays

```
DEALLOCATE (speed, STAT=ierr)
```

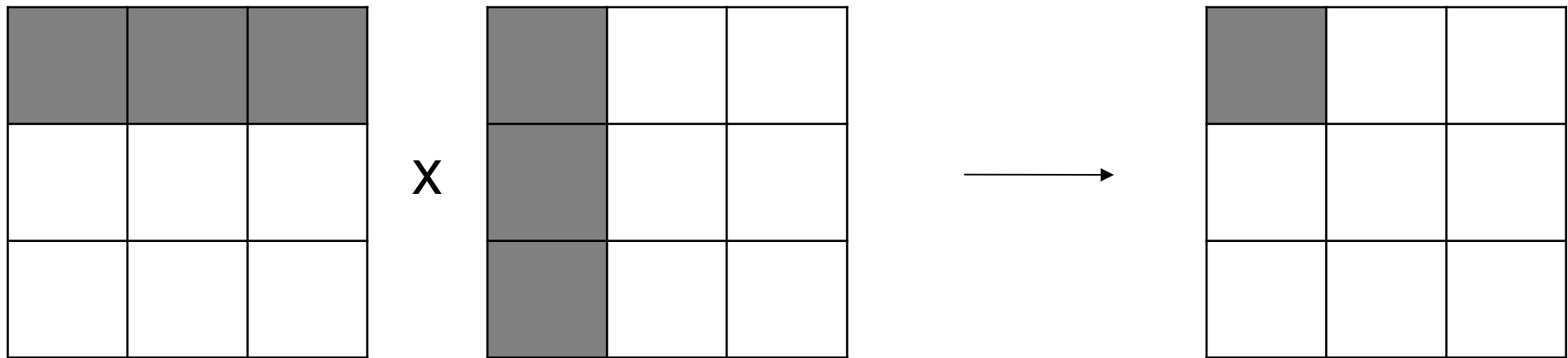
```
IF (ALLOCATED(speed)) &  
    DEALLOCATE (speed , STAT=ierr)
```



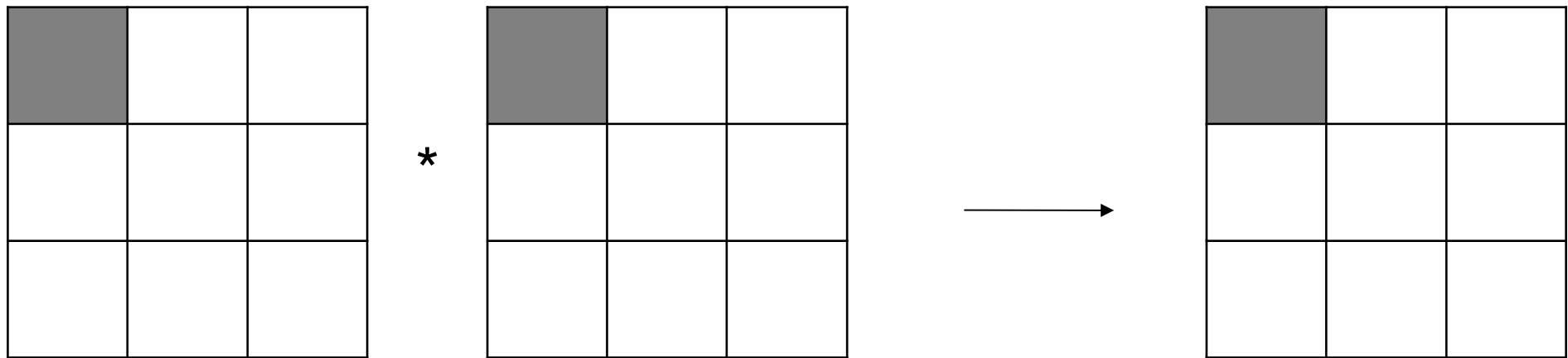
DOT_PRODUCT function



MATMUL function



multiplication operator



Practical 3

- Try the exercises on page 52



Program units

- Fortran has two main program units:
- The main program, which can contain procedures
- A module, which can contain declarations and procedures
 - Modules will be described in the next lecture



Procedures

- There are two types of procedure:
- function: a subprogram returning a result through the function name
- subroutine: a parameterised, named sub-program performing a particular task



Procedures

- Written for specific repeated tasks
- Before writing your own, look at available collections such as the:
 - Intrinsic
 - NAG Fortran Library



Intrinsic procedures

- Elemental
 - mathematical: `SIN(x)`, `LOG(x)`
 - numeric: `MAX(x1, x2)`, `CEILING(x)`
 - character: `ADJUSTL(str1)`
- Inquiry
 - array: `ALLOCATED(a)`, `SIZE(a)`
 - numeric: `PRECISION(x)`, `RANGE(x)`
- Transformational
 - array: `RESHAPE(a1, a2)`, `SUM(a)`
- Non-elemental
 - `DATE_AND_TIME`, `SYSTEM_CLOCK`



Type conversion functions

- `REAL (i)` converts the integer type value `i` to real type
- `INT (x)` converts the real type value `x` to integer type (by truncation)
- `NINT (x)` returns the integer value nearest to the real type value `x` (by rounding)



Main program syntax

```
[PROGRAM [<main program name>] ]  
<declaration of local objects>  
<executable statements>  
[ CONTAINS  
<internal procedure definitions> ]  
END [PROGRAM [<main program name>]]
```



Main program example

```
PROGRAM Main
  IMPLICIT NONE
  REAL :: x
  READ(*,*) x
  WRITE(*,"(F12.4)") Negative(x)
CONTAINS
  ! Real function Negative coded here
END PROGRAM Main
```



Function syntax

```
[<prefix>] FUNCTION <proc-name> ([<dummy  
args>])  
<declaration of dummy args>  
<declaration of local objects>  
<executable statements, assigning result to  
proc-name>  
END [FUNCTION [<proc-name>] ]
```



Function example

```
PROGRAM Main
  IMPLICIT NONE
  ! Specification part
  ! Execution part
CONTAINS
  REAL FUNCTION Negative(a)
    REAL :: a
    Negative = -a
  END FUNCTION Negative
END PROGRAM Main
```



Function example

```
PROGRAM Main
  IMPLICIT NONE
  ! Specification part
  ! Execution part
CONTAINS
  FUNCTION Negative(a)
    REAL :: a, Negative
    Negative = -a
  END FUNCTION Negative
END PROGRAM Main
```



Function facts

- A value must be assigned to the function name within the body of the function
- Side-effects must be avoided. For example do not alter the value of any argument, do not read or write values. Use a subroutine if side-effects are unavoidable.



Subroutine syntax

```
SUBROUTINE <proc-name> [ (<dummy args> ) ]  
<declaration of dummy args>  
<declaration of local objects>  
<executable statements>  
END [ SUBROUTINE [ <proc-name> ] ]
```



Subroutine example

```
PROGRAM Thingy
  IMPLICIT NONE
  ...
  CALL OutputFigures (NumberSet)
  ...
CONTAINS
  SUBROUTINE OutputFigures (Numbers)
    REAL, DIMENSION(:) :: Numbers
    WRITE (*, "(5F12.4)") Numbers
  END SUBROUTINE OutputFigures
END PROGRAM Thingy
```



Argument association

- In the invocation

```
CALL OutputFigures (NumberSet)
```

and the declaration

```
SUBROUTINE OutputFigures (Numbers)
```

`NumberSet` is the actual argument which is argument associated with the dummy argument `Numbers`

- Arguments must agree in type



Dummy argument intent

- `INTENT (IN)` can only be referenced - necessary if actual argument is a literal
- `INTENT (OUT)` must be assigned to before use
- `INTENT (INOUT)` can be referenced and assigned to



Local objects

```
REAL FUNCTION Area(x, y, z)
REAL, INTENT(IN) :: x, y, z
REAL :: height, theta ! local object
theta = ... ! Use x, y, z
height = ... ! Use theta, x, y, z
Area = ... ! Use height and y
END FUNCTION Area
```



Local objects

- are created when procedure invoked
- are destroyed when procedure completes
- do not retain values between calls



SAVE attribute

- Allows local objects to retain their values between procedure invocations

```
SUBROUTINE Barmy(arg1, arg2)
REAL, INTENT(IN) :: arg1
REAL, INTENT(OUT) :: arg2
INTEGER, SAVE :: NumInvocs = 0
NumInvocs = NumInvocs + 1
...
```



Scoping rules

- The scope of an entity is the range of program units where it is visible
- Internal procedures can inherit entities by host association
- Objects declared in modules can be made visible by use association



Host Association

```
PROGRAM CalculatePay
INTEGER :: NumberCalcsDone = 0
    ...
CONTAINS
    SUBROUTINE PrintPay(Pay, Tax)
        REAL, INTENT(IN) :: Pay, Tax
            ...
        NumberCalcsDone = ... !host assn
    END SUBROUTINE PrintPay
END PROGRAM      CalculatePay
```



Use Association

```
MODULE Tally
  INTEGER :: NumberCalcsDone
END MODULE Tally
PROGRAM CalculatePay
  USE Tally
  REAL :: GrossPay, TaxRate, Delta
  ...
  NumberCalcsDone = ... !use assn
END PROGRAM CalculatePay
```



Scope of Names

```
PROGRAM Proggie
  REAL :: A, B, C
  CALL Sub(A)
CONTAINS
  SUBROUTINE Sub(D)
    REAL :: D;    REAL :: C
    B=...;    C=...;    D=...
  END SUBROUTINE Sub
END PROGRAM Proggie
```



Dummy array arguments

- Two types of dummy array argument:
 - Explicit shape – all the bounds are specified. The actual argument must conform in size and shape.
 - Assumed shape – all the bounds are inherited from the actual argument which must conform in rank



Explicit-shape

```
REAL, DIMENSION(8,8), INTENT(IN) :: &  
    expl_shape
```

- Actual argument must be of type real, have size 64 and shape 8,8
- In this subprogram the bounds are 1:8,1:8 whatever they may be in the calling unit



Assumed-shape

```
REAL, DIMENSION (:, :), INTENT (IN) :: &  
    assum_shape
```

- Actual argument here must have rank 2
- In the subprogram the lower bounds are 1 unless another value is given, whatever they may be in the calling unit

```
REAL, DIMENSION (0:, 0:), &  
    INTENT (IN) :: assum_shape
```



External function

- An external function is defined outside the body of the program which uses it. The program needs to inform the compiler of the type of this function and that it is external.

```
REAL :: Negative
```

```
EXTERNAL :: Negative
```

```
REAL, EXTERNAL :: Negative
```



Practical 4

- Try the questions on page 67



Modules

- Constants and procedures can be encapsulated in modules for use in one or more programs



Points about modules

- Within a module, functions and subroutines are known as module procedures
- Module procedures can contain internal procedures
- Module objects can be given the `SAVE` attribute
- Modules can be `USED` by procedures and modules
- Modules must be compiled before the program unit which uses them.



Module syntax

```
MODULE module-name  
[ <declarations and specification statements> ]  
[ CONTAINS  
<module-procedures> ]  
END [ MODULE [ module-name ] ]
```



Module example

```
MODULE Triangle_Operations
  IMPLICIT NONE
  REAL, PARAMETER :: pi=3.14159
CONTAINS
  FUNCTION theta(x,y,z)
    ...
  END FUNCTION theta
  FUNCTION Area(x,y,z)
    ...
  END FUNCTION Area
END MODULE Triangle_operations
```



Using modules

```
PROGRAM TriangUser  
  USE Triangle_Operations  
  IMPLICIT NONE  
  REAL :: a, b, c
```



Restricting visibility

- The visibility of an object declared in a module can be restricted to that module by giving it the attribute `PRIVATE`

```
REAL :: Area, theta
```

```
PUBLIC                               !confirm default
```

```
PRIVATE :: theta                    !restrict
```

```
REAL, PRIVATE :: height!restrict
```



USE rename syntax

```
USE <module-name> &  
    [, <new-name> => <use-name>]
```



Use Rename example

```
USE Triangle_Operations, &  
  Space => Area
```



USE ONLY syntax

```
USE <module-name> [, ONLY : <only-list>]
```



Use Only example

```
USE Triangle_operations, ONLY: &  
    pi, Space => Area
```



DERIVED types

```
TYPE COORDS_3D
  REAL :: x, y, z
END TYPE COORDS_3D
!
TYPE(COORDS_3D) :: pt1, pt2
```



Supertypes

```
TYPE SPHERE
  TYPE(COORDS_3D) :: centre
  REAL :: radius
END TYPE SPHERE

!
TYPE(SPHERE) :: bubble, ball
```



Components of an object

- An individual component of a derived type object can be selected by using the % operator:

```
pt1%x = 3.0
```

```
ball%radius = 1.0
```

```
ball%centre%x = 0.0
```



Whole object assignment

- Use the derived type name as a constructor:

```
pt1 = COORDS_3D(3.0, 4.0, 5.0)
```

```
ball = SPHERE(centre=pt1, radius=5.0)
```



Input or Output

- Components are accessed in defined order, for example:

```
ball%centre%x
```

```
ball%centre%y
```

```
ball%centre%z
```

```
ball%radius
```



True portability

- The range and precision of numeric values are not defined in the language but are dependent on the computer system used
- For integers, `RANGE (i)`, and for reals `RANGE (x)` return the range of values supported
- For reals, `PRECISION (x)` returns the precision to which values are held



Properties of integers

- Integer values are always stored exactly so it is only necessary to define their range.
- The intrinsic function `SELECTED_INT_KIND (<range>)`
- returns an integer `KIND` value which can be used to declare integers of this kind.



Integers of chosen kind

```
INTEGER, PARAMETER :: &  
    ik9 = SELECTED_INT_KIND(9)  
INTEGER(KIND=ik9) :: i
```

- `ik9` is non-negative if the desired range of integer values, $-10^9 < n < 10^9$ can be achieved



Properties of reals

`SELECTED_REAL_KIND &`
`(<precision>, <range>)`

- returns an integer `KIND` value which can be used to declare reals with the chosen properties
- It returns -1 if the precision cannot be achieved, and -2 if the range cannot be achieved



Reals of chosen kind

```
INTEGER, PARAMETER :: &  
    rk637 = SELECTED_REAL_KIND(6,37)  
REAL(KIND=rk637) :: x
```



Constants and KIND

```
INTEGER(KIND=ik9) :: I = 7_ik9
```

```
REAL(KIND=rk637) :: x = 5.0_rk637
```



Practical 5

- Try the questions on page 77



Bibliography

Fortran95/2003 explained
Michael Metcalf, John Reid, Malcolm Cohen.
Oxford University Press
ISBN 0 19 852693 8

Fortran 90 Programming
T.M.R.Ellis, Ivor R.Philips, Thomas M.Lahey
Addison-Wesley
ISBN 0-201-54446-6

Fortran 90/95 for Scientists and Engineers
Stephen J.Chapman
McGraw Hill
ISBN 007-123233-8

