Introductory Fortran Programming

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Outline

List of Topics

Contents

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- Gentle introduction to Fortran 77 and 95 programming
- File I/O
- Arrays and loops
- Functions and subroutines
- Detailed explanation of modules
- Computational efficiency aspects
- Using modules as objects

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About learning Fortran

- Fortran is a less complicated language than C++ and Java
- Even so it takes time to master the advanced details of Fortran 95
- At least 6 months to a year working with Fortran 95 before you are familiar with most of the details
- Four days can only get you started
- You need to use Fortran 95 in your own projects to master the language
- Fortran 77 code is not the main topic here, but you need to have some knowledge of it

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Fortran 77

- Into the early/middle of the nineties Fortran 77 was the dominating language for number crunching
- The predecessor Fortran IV was replaced by Fortran 77 in the early eighties
- At IBM in 1954 a group of people started to design the FORmula TRANslator System, or FORTRAN0
- The first version of Fortran was released in 1957 and the language has evolved over time
- Like many procedural languages Fortran has a fairly simple syntax
- Fortran is good for only one thing: NUMBERCRUNCHING

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Fortran 95

- Fortran 95 extends Fortran 77 with
  - Nicer syntax, free format instead of fixed format
  - User defined datatypes using the TYPE declaration
  - Modules containing data definitions and procedure declarations
  - No implicit variable declarations, avoiding typing errors

Fortran versus other languages

- C is low level and close to the machine, but can be error prone
- C++ is a superset of C and more reliable
- Java is simpler and more reliable than C++
- Python is more high-level than Java
- Fortran 95 is more reliable than Fortran 77

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Why these differences

- There are some reasons why som languages are faster than others
  - The structure and complexity of the language
  - The complexity of the CPU and the experience of the compiler developers
  - Compilation vs. interpretation

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Some guidelines

- Fortran 77 gives very fast programs, but the source code is less readable and more error prone due to implicit declarations
- Use Fortran 95 for your main program and if speed is critical use Fortran 77 functions
- Sometimes the best solution is a combination of languages, e.g. Fortran with Python or C++
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Our first Fortran 77 program

- Goal: make a program writing the text “Hello World
- Implementation
  - Without declaring a text string variable
  - With a text string variable declaration

Without declaring a string variable

- Fortran fixed format

```
C234567
      PROGRAM hw1
         WRITE(*,*) 'Hello World'
      END PROGRAM hw1
```

With declaring a string variable

- Fortran fixed format

```
C234567
      PROGRAM hw1
         CHARACTER*11 str = 'Hello World'
         WRITE(*,*) str
      END PROGRAM hw1
```

Some comments to the “Hello World program

- Fortran 77 uses fixed format
- The source code is divided into positions on the line
- This is a heritage from the old days when communication with the computer was by punched cards
- A character in the first column identifies to the compiler that the rest of the line is a comment
- The coumns 2 to 5 is for jump labels and format specifiers
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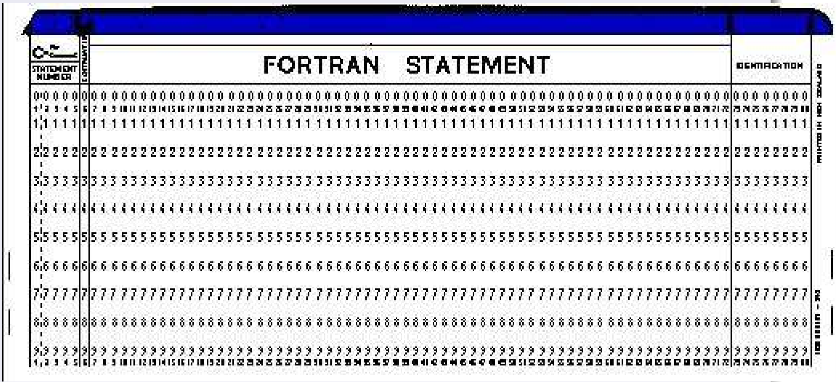
An example of a punched card for Fortran

- the layout of a Fortran card



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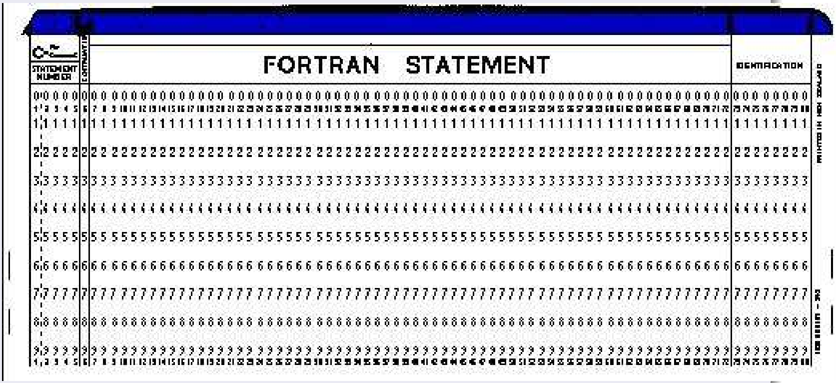
  - 

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Scientific Hello World in Fortran 95

- Usage:

```
./hw1 2.3
```

- Output of the program hw1

```
Hello, World! sin(2.3)=0.745705
```

- What to learn
  - Store the first command-line argument in a floating-point variable
  - Call the sine function
  - Write a combination of text and numbers to the screen

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The code

- The hw1 program

```
PROGRAM hw1
   IMPLICIT NONE
   DOUBLE PRECISION  :: r, s
   CHARACTER(LEN=80) :: argv ! Input argument
   CALL getarg(1,argv)       ! A C-function
   r = a2d(argv)             ! Our own ascii to
                             ! double
   s = SIN(r)                ! The intrinsic
                             ! SINE function
   PRINT *, 'Hello Word sin(',r,')=',s
END PROGRAM hw1
```

Dissection(1)

- Contrary to C++ the compiler does not need to se a declaration of subroutines and intrinsic functions
- Only external functions must be declared
- Comments in Fortran 95 are the exclamation mark *!* on a line
- The code is free format unlike Fortran 77

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Dissection(2)

- Floating point variables in Fortran
  - REAL: single precision
  - DOUBLE PRECISION: double precision
- a2d: your own ascii string to double conversion function, Fortran has no intrinsic functions of this kind in contrast to C/C++ so you have to write this one yourself or you can use the C/C++ atof() if you declare it as external real function
- Automatic type conversion: DOUBLE PRECISION = REAL
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An interactive version

- Let us ask the user for the real number instead of reading it from the command line

```
WRITE(*.FMT='(A)',ADVANCE='NO') 'Give a number: '
READ(*,*) r
s = SIN(r)
! etc.
```

- The keyword *ADVANCE='NO'* suppress the linefeed Fortran put at the end of each *WRITE* statement

Scientific Hello World in Fortran 77

- The f77 code

```
C234567
      PROGRAM hw1
        REAL*8 r,s
        CHARACTER*80 argv
        CALL getarg(1,argv)
        r = a2d(argv)
        s = SIN(r)
        WRITE(*,*)'Hello World! sin(',r')=',s
      END PROGRAM hw1
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Differences from the Fortran 95 version

- Fortran 77 uses REAL*8 instead of DOUBLE PRECISION
- Fortran 77 lacks IMPLICIT NONE directive
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How to compile and link (Fortran 95) on a unix/linux system

- One step (compiling and linking):

```
unix> f90 -O3 -o hw1 hw1.f90
```

- Two steps:

```
unix> f90  -O3 -c hw1.f90
unix> f90 -O3 -o hw1 hw1.o
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- A linux system with Intel Fortran Compiler:

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How to compile and link (Fortran 95) on a windows system

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- This *IDE* contains drop down menus to compile and run the program
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Using the make utility to compile a program

- What is the make utility?
  - The make utility reads a file containing the name(s) of the file(s) to be compiled togehter with the name of the executable program
- The makefile is either called makefile or Makefile as default and is available on all unix/linux systems
- Invoking the make utiltity:

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linux> make
unix> make
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- On unix machines there are often both the gnu make utility and a native make. The native make utility can often have a different syntax than the gnu make

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A short example of a makefile

- Makefile

```
$(shell ls *.f90 ./srclist)
SRC=$(shell cat ./srclist)
OBJECTS= $(SRC:.f90=.o)
prog : $(OBJECTS)
	$(FC) -o $@ $(OBJECTS)
%.o : %.f90
	$(FC) -c $?
```

Rolling your own make script

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The looks of a make.sh script(1)

- make.sh

```
#!/bin/sh
if [ ! -n ``$F90_CMPL'' ]; then
  case `uname -s` in
    Linux)
       F90_CMPL=ifort
       F90_OPTS= -static
       ;;
    *)
       F90_CMPL=f90
       F90_OPTS=
  esac
fi
```

The looks of the make.sh script(2)

- make.sh

```
files=‘/bin/ls *.f90‘
for file in files; do
 stem=‘echo $file | sed ’s/\.f90//’‘
 echo $F90_CMPL $F90_OPTS -I. -o $stem $file
 $F90_CMPL $F90_OPTS -I. -o $stem $file
 ls -s stem
```

How to compile and link (Fortran 77)(1)

- Either use the f90 compiler or if present the f77 compiler
- Rememeber that Fortran 77 is s subset of Fortran 95
- An example:

```
f90 -o prog prog.f or
f77 -o prog prog.f
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How to compile and link (Fortran 77) (2)

- NOTE! The file extension of the Fortran source code is important
- A file with the extension *.f90* is automatically a Fortran 90/95 free format file
- If the file has the extension *.f* the compier sees this as a Fortran 77 fixed format file

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How to compile and link in general

- We compile a set of programs in Fortran and C++
- Compile each set of files with the right compiler:

```
unix> f90 -O3 -c *.f90
unix> g++ -O3 -c *.cpp
```

- Then link:

```
unix> f90 -o exec_file  *.o -L/some/libdir \
      -L/other/libdir -lmylib -lyourlib
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- Library type: lib*.a: static; lib*.so: dynamic

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List of Topics

Example: Data transformation

- Suppose we have a file with an xy-data pair

```
0.1 1.1
0.2 1.8
0.3 2.2
0.4 1.8
```

- We want to transform the y value using some mathematical function f(y)
- Goal: write a Fortran 95 program that reads the xy-data pair from the file, transforms the y value and write the new xy-data pair to a new file

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Program structure

- Read the names of input and output files as command-line arguments
- Print error/usage message if less than two command-line arguments are given
- Open the files
- While more data in the file:
- Close the files

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- Close the files

The fortran 95 code(1)

- Code

```
FUNCTION myfunc(y) RESULT(r)
   IMPLICIT NONE
   DOUBLE PRECISION, INTENT(IN) :: y
   DOUBLE PRECISION             :: r
   IF(y>=0.) THEN
      r = y**0.5*EXP(-y)
   ELSE
      r = 0.
   END IF
END FUNCTION myfunc
```

The fortran 95 code(2)

- Code

```
PROGRAM dtrans
   IMPLICIT NONE
   INTEGER                :: argc, rstat
   DOUBLE PRECISION       :: x, y
   CHARACTER(LEN=80)      :: infilename, outfilename
   INTEGER,PARAMETER      :: ilun = 10
   INTEGER,PARAMETER      :: olun = 11
   INTEGER, EXTERNAL      :: iargc
   argc = iargc()
   IF (argc < 2) THEN
      PRINT *, 'Usage: dtrans infile outfile'
      STOP
   END IF
   CALL getarg(1,infilename)
   CALL getarg(2,outfilename)
```

The fortran 95 code(3)

- Code

```
OPEN(UNIT=ilun,FILE=infilename, &
  FORM='FORMATTED', IOSTAT=rstat)
  OPEN(UNIT=olun,FILE=outfilename,&
  FORM='FORMATTED', IOSTAT=rstat)
  rstat = 0
  DO WHILE(rstat == 0)
    READ(UNIT=ilun,FMT='(F3.1,X,F3.1)',&
         IOSTAT=rstat) x, y
    IF(rstat /= 0) THEN
      CLOSE(ilun); CLOSE(olun)
      STOP
    END IF
    y = myfunc(y)
    WRITE(UNIT=olun,FMT='(F3.1,X,F3.1)',&
          IOSTAT=rstat) x, y
  END DO
END PROGRAM dtrans
```

List of Topics

Fortran file opening

- Open a file for reading

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OPEN(UNIT=ilun,FORM='FORMATTED',IOSTAT=rstat)
```

- Open a file for writing

```
OPEN(UNIT=ilun,FORM='FORMATTED',IOSTAT=rstat)
```

- Open for appending data

```
OPEN(UNIT=ilun,FORM='FORMATTED',&
     POSITION='APPEND',IOSTAT=rstat)
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Fortran file reading and writing

- Read a double precision number

```
READ(UNIT=ilun,FMT='(F10.6)',IOSTAT=rstat) x
```

- Test if the reading was successful

```
IF(rstat /= 0) STOP
```

- Write a double precision number

```
WRITE(UNIT=olun,FMT='(F20.12)',IOSTAT=rstat) x
```

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Formatted output

- The formatted output in Fortran is selected via the FORMAT of FMT statement
- In fortran 77 the FORMAT statement is used

```
C234567
 100  FORMAT(F15.8)
      WRITE(*,100) x
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- In Fortran 95 the FMT statement is used

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WRITE(*,FMT='(F15.8)') x
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- In Fortran 95 the FMT statement is used

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WRITE(*,FMT='(F15.8)') x
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A convenient way of formatting in Fortran 95(1)

- Instead of writing the format in the FMT statement we can put it in a string variable

```
CHARACTER(LEN=7)  :: fmt_string
fmt_string = '(F15.8)'
WRITE(*,FMT=fmt_string) x
```

A convenient way of formatting in Fortran 95(2)

- We can use a set of such format strings

```
CHARACTER(LEN=7),DIMENSION(3)  :: fmt_string
fmt_string(1) = '(F15.8)'
fmt_string(2) = '(2I4)'
fmt_string(3) = '(3F10.2)'
WRITE(*,FMT=fmt_string(1)) x
```

Unformatted I/O in Fortran

- More often than not we use huge amount of data both for input and output
- Using formatted data increase both the filesize and the time spent reading and writing data from/to files
- We therefore use unformatted data in these cases

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Opening and reading an unformatted file

- Open syntax:

```
OPEN(UNIT=ilun,FILE=infile,FORM='UNFORMATTED',&
     IOSTAT=rstat)
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- Reading syntax:

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READ(UNIT=ilun,IOSTAT=rstat) array
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- the array variable can be a single variable, a vector or a multidimensional matrix

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- This is performed by using direct access file I/O
- Open syntax:

```
OPEN(UNIT=ilun,FILE=infile,ACCESS='DIRECT',&
     RECL=lng,IOSTAT=rstat)
```

- Reading syntax:

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READ(UNIT=ilun,REC=recno,IOSTAT=rstat) array
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- The array most be of equal size to the record length and the recno variable contains the record number to be read
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The namelist file

- A special type of file exists in Fortran 95
- It is the namelist file which is used for input of data mainly for initializing purposes
- Reading syntax:

```
INTEGER :: i, j, k
NAMELIST/index/i, j, k
READ(UNIT=ilun,NML=index,IOSTAT=rstat)
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- This will read from the namelist file values into the variables i, j, k

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The contents of a namelist file

- Namelist file syntax:

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&index i=10, j=20, k=4 /
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- A namelist file can contain more than one namelist

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List of Topics

Matrix-vector product

- Goal: calculate a matrix-vector product
  - Make a simple example with known solution (simplifies debugging)
  - Declare a matrix A and vectors x and b
  - Initialize A
  - Perform $b = A * x$
  - Check that b is correct

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Basic arrays in Fortran

- Fortran 77 and 95 uses the same basic array construction
- Array indexing follows a quickly learned syntax:

  ```
  q(3,2)
  ```

- This is the same as in Matlab. Note that in C/C++ a multidimensional array is transposed

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Declaring basic vectors

- Declaring a fixed size vector

```
INTEGER, PARAMETER                :: n = 100
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DOUBLE PRECISION, DIMENSION(50)   :: b
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- Vector indices starts at 1 not 0 like C/C++

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INTEGER, PARAMETER                  :: n = 100
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```

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Declaring basic matrices

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INTEGER, PARAMETER                    :: n = 100
DOUBLE PRECISION, DIMENSION(m,n) :: x
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Looping over the matrix

- A nested loop

```
INTEGER    :: i, j
DO j = 1, n
  DO i = 1, n
    A(i,j) = f(i,j) + 3.14
  END DO
END DO
```

Matrix storage scheme

- Note: matices in fortran are stored column wise; the row index should vary fastest
- Recall that in C/C++ matrices are stored row by row and the column index should vary fastest
- Typical loop in C/C++ (2nd index in inner loop):

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- Very often we do not know the length of the array in advance
- By using dynamic memory allocation we can allocate the necessary chunk of memory at runtime
- You need to allocate and deallocate memory

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Dynamic memeory allocation in Fortran 95

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- Using the ALLOCATABLE attribute
- Using a POINTER variable

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Allocating memory using the ALLOCATABLE attribute

- Declare an ALLOCATABLE array variable

```
DOUBLE PRECISION, ALLOCATABLE, DIMENSION(:) :: x
ALLOCATE(x(100))
  ...
DEALLOCATE(x)
```

Allocating memory using a POINTER

- Declare a pointer array variable

```
DOUBLE PRECISION, POINTER  :: x(:)
ALLOCATE(x(100))
  ...
DEALLOCATE(x)
```

- Keep in mind that a Fortran 95 POINTER is not the same as a pointer in C/C++

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Declaring and initializing A, x and b

- Code

```
DOUBLE PRECISION, POINTER :: A(:,:), x(:), b(:)
CHARACTER(LEN=20)         :: str
INTEGER                   :: n, i, j
CALL getarg(1,str)
n = a2i(str)
ALLOCATE(A(n,n)); ALLOCATE(x(n))
ALLOCATE(b(n))
DO j = 1, n
  x(j) = j/2.
  DO i = 1, n
    A(i,j) = 2. + i/j
  END DO
END DO
```

Matrix-vector product loop

- Code for computation of the matrix-vector product

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DOUBLE PRECISION          :: sum
DO j = 1, n
  sum = 0.
  DO i = 1, n
    sum = sum + A(i,j) * x(i)
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```

- Another way to compute eth matrix-vector product is to use an intrinsic fortran function *MATMUL*

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List of Topics

Subroutines

- A subroutine does not return any value and is the same as a void function in C/C++
- In Fortran all arguments are passed as the address of the variable in the calling program
- This is the same as a call by refrence in C++
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An example of a subroutine

- This subroutine will calculate the square root of two arguments and returning the sum of the results in a third argument

```
SUBROUTINE dsquare(x,y,z)
  DOUBLE PRECISION, INTENT(IN)  :: x, y
  DOUBLE PRECISION, INTENT(OUT) :: z
  z = SQRT(x) + SQRT(y)
END SUBROUTINE dsquare
```

- Using the INTENT(IN) and INTENT(OUT) will prevent any accidentally changes of the variable(s) in the calling program by flagging an error at compile time

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An example of a function in Fortran 77 style

- This function will calculate the square root of two arguments and returning the sum of the results

```
C234567
      DOUBLE PRECISION, FUNCTION dsquare(x,y)
        DOUBLE PRECISION, INTENT(IN)  :: x, y
        DOUBLE PRECISION              :: z
        z = SQRT(x) + SQRT(y)
        dsquare = z
      END FUNCTION dsquare
```

An example of a function in Fortran 95 style

- This function will calculate the square root of two arguments and returning the sum of the results

```
FUNCTION dsquare(x,y), RESULT(z)
  DOUBLE PRECISION, INTENT(IN)  :: x, y
  DOUBLE PRECISION              :: z
  z = SQRT(x) + SQRT(y)
END FUNCTION dsquare
```

- It is the variable type in the RESULT statement that identifies the type of the function

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List of Topics

More about pointers in Fortran 95

- As mentioned earlier a pointer in Fortran 95 *IS NOT* the same as a pointer in C/C++
- A fortran 95 pointer is used as an alias pointing to another variable, it can be a single variable, a vector or a multidimensional array
- A pointer must be associated with a target variable or another pointer and have the same shape that the target it is pointing to
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Some examples of pointer usage(1)

- A target pointer example

```
DOUBLE PRECISION, TARGET, DIMENSION(100) :: x
DOUBLE PRECISION, POINTER                :: y(:)
 ...
y => x
 ...
y => x(20:80)
 ...
y => x(1:33)
NULLIFY(y)
```

Some examples of pointer usage(2)

- What happens when we try to access a deallocated array?

```
PROGRAM ptr
   IMPLICIT NONE
   DOUBLE PRECISION, POINTER :: x(:)
   DOUBLE PRECISION, POINTER :: y(:)
   ALLOCATE(x(100))
   x = 0.
   x(12:19) = 3.14
   y => x(10:20)
   PRINT '(A,3F10.4)', 'Y-value ', y(1:3)
   y => x(11:14)
   DEALLOCATE(x)
   PRINT '(A,3F10.4)', 'Y-value ', y(1:3)
   PRINT '(A,4F10.4)', 'X-value ', x(11:14)
END PROGRAM ptr
```

Some examples of pointer usage(3)

- This is what happened

```
bullet.uio.no$ EXAMPLES/ptr
    0.0000     0.0000     3.1400
    0.0000     3.1400     3.1400
forrtl: severe (174): SIGSEGV,
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- When we try to access the x-array in the last PRINT statement we get an segmentation fault
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- In our little example we clearly see that the memory pointed to by the x-array is no longer available
- On the other hand the part of the memory the y-array is pointing to is still available
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List of Topics

Exercise1: Modify the Fortran 95 Hello World program

- Locate the Hello World program
- Compile the program and test it
- Modification: write "Hello World!" and format it so the text and numbers are without unnecessary spaces and trailing zeroes

```
Hello World sin(    2.3000000000000      )=   0.7457052121
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- Locate the first Hello World program
- Read the three command-line arguments: *start*, *stop* and *inc*
- Provide a “usage message and abort the program in case there are too few command-line arguments
- Do r = loop_start, loop_stop, loop_inc and compute the sine of r and write the result
- Write and additional loop using DO WHILE construction
- Verify that the program works

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Exercise3: Integrate a function(1)

- Write a function

```
DOUBLE PRECISION FUNCTION trapezoidal(f,a,b,n)
  DOUBLE PRECISION, EXTERNAL :: f
  DOUBLE PRECISION           :: a, b
  INTEGER                    :: n
  ...
END FUNCTION trapezoidal
```

- It shall integrate a user-defined function
  $\int_a^b f(x)\,\mathrm{d}x \approx h(\frac{f(a)}{2} + \frac{f(b)}{2} + \sum_{i=1}^{n-1} f(a+ih)), h = \frac{b-a}{n-1}$

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Exercise3: Integrate a function(2)

- The user defined function is specified as *external* in the argument specifications of the trapezoidal function
- Any function taking a double precision as an argument and returning a double precision number can now be used as an input argument to the trapezoidal function
- Verify that *trapeziodal* is implemented correctly

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Binary format

- A number like π can be represented in ASCII format as 3.14 (4 bytes) or $3.14159E+00$ (11 bytes), for instance
- In memory, the number occupies 8 bytes (a *double*), this is the binary format of the number
- The binary format (8 bytes) can be stored directly in a file
- Binary format (normally) saves space, and input/output is much faster since we avoid translation between ASCII characters and the binary representation
- The binary format varies with the hardware and occasionally with the compiler version
- Two types of binary formats: little and big endian
- Motorola and Sun: big endian; Intel and HP Alpha: little endian

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Exercise 4: Work with binary data in Fortran 77 (1)

- Scientific simulations often involve large data sets and binary storage of numbers saves space in files
- How to write numbers in binary format in Fortran 77:

```
WRITE(UNIT=olun) array
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- Create datatrans2.f (from datatrans1.f) such that the input and output data are in binary format
- To test the datatrans2.f we need utilities to create and read binary files
  - make a small Fortran 77 program that generates *n* xy-pairs of data and writes them to a file in binary format (read *n* from the command line)
  - make a small Fortran 77 program that reads xy-pairs from a binary file and writes them to the screen
- With these utiltities you can create input data to datatrans2.f and view the file produced by datatrans2.f

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Exercise 4: Work with binary data in Fortran 77 (3)

- Modify datatrans2.f program such that the x and y numbers are stored in one long dynamic array
- The storage structure should be x1, y1, x2, y2, ...
- Read and write the array to file in binary format using one READ and one WRITE call
- Try to generate a file with a huge number (10 000 000) of pairs and use the unix *time* command to test the efficiency of reading/writing a single array in one READ/WRITE call compared with reading/writing each number separately

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Exercise 5: Work with binary data in Fortran 95

- Do the Fortran 77 version of the exercise first!
- How to write numbers in binary format in Fortran 95

```
WRITE(UNIT=olun, IOSTAT=rstat) array
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- Modify datatrans1.f90 program such that it works with binary input and output data (use the Fortran 77 utilities in the previous exercise to create input file and view output file)

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Exercise 6: Efficiency of dynamic memory allocation(1)

- Write this code out in detail as a stand-alone program:

```
INTEGER, PARAMETER  ::  nrepetitions = 1000000
INTEGER             :: i, n
CHARACTER(LEN=80)   :: argv
CALL getarg(1,argv)
n = a2i(argv)
DO i = 1, nrepetitions
  ! allocate a vector of n double precision numbers
  ! set second entry to something
  ! deallocate the vector
END DO
```

Exercise 6: Efficiency of dynamic memory allocation(2)

- Write another program where each vector entry is allocated separately:

```
INTEGER          :: i, j
DOUBLE PRECISION :: sum
DO i = 1, nrepetitions
  ! allocate each of the double precision
  !numbers separately
  DO j = 1, n
    ! allocate a double precision number
    ! add the value of this new item to sum
    ! deallocate the double precision number
  END DO
END DO
```

Exercise 6: Efficiency of dynamic memory allocation(3)

- Measure the CPU time of vector allocation versus allocation of individual entries:

```
unix> time myprog1
unix> time myprog2
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- Adjust the nrepetitions such that the CPU time of the fastest method is of order 10 seconds

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