Numerical Modelling in FORTRAN day 2

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Goals for today

- Review main points in online materials you read for homework
  - http://www.cs.mtu.edu/%7eshene/COURSES/cs201/NOTES/intro.html
- More details about loops
- Finite difference approximation
- Introduce and practice
  - subroutines & functions
  - arrays

```
program miscellaneous_things
  implicit none
  integer i,j
  real a
  logical equal

  i=2; j=5   ! multiple statements on same line

  ! continuing statements over several lines
  a = 2*i +    &
       3*j

  ! careful with integer constants!
  print*,2/3, 2./3, 2/3. , 2.0/3.0

  ! example use of logical variables
  equal = (i==j)
  print*,equal

  ! use of mod(), min() and max() functions
  do i = 1,10
     print*,mod(i,3),min(i,j),max(i,j)
  end do

  ! real->integer conversion functions
  do i = -8,8
     a = real(i)/4.
     print*,a,int(a),nint(a),floor(a),ceiling(a)
  end do

end program miscellaneous_things
```

Miscellaneous things

- Continuing lines:
  - f95 use ‘&’ at the end of the line
  - f77: put any character in column 6 on next line
- Formats of constants:
  - Use ‘.’ to distinguish real from integer (avoid 2/3=0 !)
  - 1.234×10^{-13} is written as 1.234e-13
- logical variables have 2 values: .true. or .false.
- Variable naming rules:
  - start with letter
  - mix numbers, letters and _
  - no spaces

Character/string definitions

- character :: a   (single character)
- character(len=10) :: a   (string of length 10)
- character :: a*10, b*5
- character*15:: a,b   (fortran77 style)
- character(len=*) :: Name= ‘Paul’
  - automatic length, otherwise strings will be truncated or padded with spaces to fit declared length

Initialising variables

- Always initialise variables! Don’t assume they will automatically be set to 0!
- Either
  - when defined, e.g., real:: a=5.
  - in the program, e.g., a=5.0
  - read from keyboard or file

Arithmetic operators

- e.g., what does a+b*c**3 mean?
  - ((a+b)*c)**3? a+(b*c)**3? etc.
  - No! correct is: a+(b*(c**3))
  - priority is **, (* or /) then (+ or -)
- Also LOGICAL operators, in this priority:
  - .not., .and., .or., (.eqv. or .neqv.)
- Be careful mixing variable types (e.g. integer & real) in the same expression!

Some intrinsic mathematical functions

- abs (absolute value, real or integer)
- sqrt (square root)
- sin, cos, tan, asin, acos, atan, atan2: assume angles are in **radians**
- exp and log : log is **natural log**, use log10 for base 10.
- also cosh, sinh, tanh
- for full list see a manual

Some conversion functions

- Int(a): round to smaller # (4.7->4; -4.6->-4)
- Nint(a): nearest integer (4.7->5; -4.6->-5)
- Floor(a): (4.7->4; -4.6->-5)
- Ceiling(a): (4.7->5; -4.6->-4)
- Float(i): integer -> real
- Real(c): real part of complex
- mod(a,b) is remainder of x-int(x/y)*y
- max(a,b,c,….), min(a,b,c,…)

read(*,*) and write(*,*)

- read(*,*) and write(*,*) do the same thing as read* and print* but are more flexible:
  - The 1st * can be changed to a file number, to read or write from a file
  - The 2nd * can be used to specify the format (e.g., number of decimal places)
- More about this later in the course!

do loops: more types

```
program more_loops
  implicit none
  integer :: j

  print*,'first loop'
  do j = 0,10,2        ! 0 to 10 in steps of 2
     write(*,*) j      ! this does the same as print*
  end do

  print*,'second loop'
  do j = 10,0,-1        ! steps of -1
     print*,j
  end do

  print*,'third loop'
  do     ! an infinite loop, unless you EXIT
     print*,'input 1 to exit'
     read(*,*) j                  ! does the same as read*,
     if (j==1) exit               ! single line if statement
  end do

  print*,'fourth loop'
  do while (j==1)
     print*,'input something other than 1 to exit'
     read*, j
  end do

end program more_loops
```

functions and subroutines

- Useful for performing tasks that are performed more than once in a program and/or
- Modularising (splitting up into logical chunks) the code to make it more understandable
- A function returns a value, a subroutine doesn’t (except through changing its arguments)

example functions

```
integer function sum3(a,b,c)
  implicit none
  integer,intent(in):: a,b,c ! intent is optional
                             !  but avoids bugs
  sum3 = a+b+c
end function sum3

!------------------------------

integer function factorial(n)
  implicit none
  integer,intent(in) :: n   ! the argument
  integer :: i,a            ! local variables

  a = 1
  do i=1,n ; a=a*i; enddo   ! multiple statements
                       ! "enddo" or "end do" same

  factorial = a
end function factorial
```

same thing as subroutines (less elegant)

```
subroutine sum3(a,b,c,result)
  implicit none
  real,intent(in):: a,b,c   ! intent is optional
  real,intent(out)::result !  but avoids bugs

  result = a+b+c
end subroutine sum3

!------------------------------

subroutine factorial(n,result)
  implicit none
  integer,intent(in) :: n    ! the arguments
  integer,intent(out):: result
  integer :: i,a             ! local variables

  a = 1
  do i=1,n ; a=a*i; enddo    ! multiple statements
                           ! "enddo" or "end do" same

  result = a
end subroutine factorial
```

Internal vs. external functions

- **Internal** functions (f90-) are **contained** within the program, and therefore the compiler can link them easily
- **External** functions are defined outside the main program, so the calling routine must declare their type (e.g., integer, real).
  - In f90 it is also possible to specify the type of all the arguments, using an **explicit interface block**, which has various advantages.

Example internal function

```
program funcdemo1
  implicit none
  integer :: n=0

  do while (n<1)     ! repeats until input is valid
     print*,'Input a positive integer:'
     read*,n
  end do
  print*,n,'! =',factorial(n)

contains ! this is a key statement

  integer function factorial(n)
    implicit none
    integer,intent(in) :: n
    integer :: i,a
    a = 1
    do i=1,n
       a=a*i
    enddo
    factorial = a
  end function factorial
end program funcdemo1
```

…and as an external function

```fortran
program funcdemo1
  implicit none
  integer :: n=0
  integer,external:: factorial      ! note this!

  do while (n<1)     ! repeats until input is valid
     print*,'Input a positive integer:'
     read*,n
  end do
  print*,n,'! =',factorial(n)

end program funcdemo1

integer function factorial(n)
  implicit none
  integer,intent(in) :: n
  integer :: i,a
  a = 1
  do i=1,n
     a=a*i
  enddo
  factorial = a
end function factorial
```

Arrays

```
program array_declarations
  implicit none

  real,dimension(5,5) :: a,b     ! good if several the same size
  real :: c(3,5,7), d(-5:5), e(0:1) ! good if different sizes
  integer,allocatable:: f(:),g(:,:,:) ! size is allocate in code
  integer n(3),i

  write(*,'(a,$)') 'Input 3 array dimensions:'
  read*,(n(i),i=1,3)                    ! implicit do loop
  allocate( f(n(1)), g(n(1),n(2),n(3)) )

  ! main body of the program goes here

  deallocate (f,g) ! free up memory

end program array_declarations

!----------------------------------------

real function sum1Darray (a,n)
  implicit none
  integer,intent(in):: n  ! arguments
  real,intent(in):: a(n)
  integer i               ! local variables
  real :: sum=0

  do i=1,n
     sum=sum + a(i)
  end do
  sum1Darray = sum
end function sum1Darray
```

Notes

- Indices start at 1 and go up to the declared value, e.g., if declare a(5) then it has components a(1),a(2)…a(5)
- To get a different lower index, e.g., a(-5:5)
- In subroutines&functions an argument can be used to dimension arrays
- In allocate statements other variables can be used
- Use of the (a,$) format in write avoids carriage return at the end
- Note implicit do loop n(j),j=1,3

Homework

- At the ‘Fortran 90 Tutorial’ at http://www.cs.mtu.edu/%7eshene/COURSES/cs201/NOTES/fortran.html
- Read through the sections
  - Selective Execution
  - Repetitive Execution
  - Functions (not modules - yet)
- Do the exercises on the next slides and hand in by email (.f90 files)

Exercise 1: statements & loops

- Write statements to
  - Declare a string of length 15 characters
  - Declare an integer parameter = 5
  - Declare a 1-dimensional array with indices running from -1 to +10
  - Declare a 4-dimensional allocatable array
  - Convert a real number to the nearest integer
  - Calculate the remainder after a is divided by b
- Write loops to
  - Add up all even numbers from 12 to124
  - Test each element of array a(1:100) starting from 1; if the element is positive print a message to the screen and leave the loop

Exercise 2: Mean and standard deviation

- Convert your mean & stddev program from last week into a **function** or **subroutine** that operates on a 1-D array passed in as an argument.
- Write a main program that
  - asks for the number of values,
  - allocates the array,
  - reads the values into the array,
  - calls the function you wrote and
  - prints the result
- A function can’t return both mean & stddev, so one of them will have to be an argument

Derivatives using finite-differences

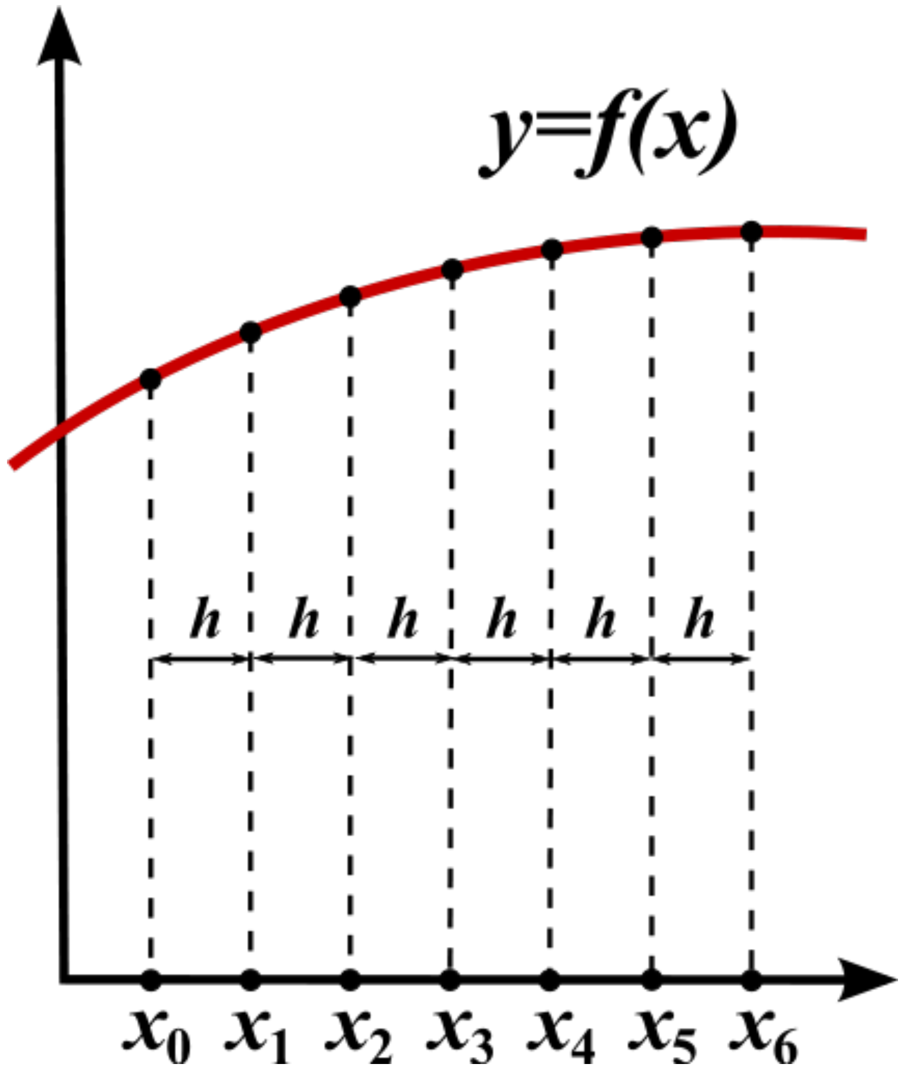
- Graphical interpretation: df/dx(x) is slope of (tangent to) graph of f(x) vs. x
- Calculus definition:

$$\frac{df}{dx} \equiv f'(x) \equiv \lim_{dx \to 0} \frac{f(x+dx) - f(x)}{dx}$$

- Computer version (finite differences):

$$f'(x) = \frac{f(x_2) - f(x_1)}{x_2 - x_1}$$

Finite Difference grid in 1-D



- Grid points x_0, x_1, x_2…x_N
  - Here xi=x_0+i*h
- Function values y_0, y_1, y_2…y_N
  - Stored in array y(i)
- (Fortran, by default, starts arrays at i=1, but you can change this to i=0)

$$\left(\frac{dy}{dx}\right)_i \approx \frac{\Delta y}{\Delta x} = \frac{y(i+1)-y(i)}{h}$$

Concept of Discretization

- True solution to equations is continuous in space and time
- In computer, space and time must be discretized into distinct units/steps/points
- Equations are satisfied for each unit/step/point but not necessarily inbetween
- Numerical solution approaches true solution as number of grid or time points becomes larger

```fortran
program Deriv1
  implicit none
  integer            :: n,i
  real,allocatable:: y(:),dydx(:)
  real               :: x,dx

  write(*,'(a,$)') 'Input number of grid points:'; read*,n
  allocate (y(n),dydx(n))   ! allocate grid arrays

  dx = 10.0/(n-1)   ! grid spacing, assuming x from 0->10
  do i = 1,n
     x = (i-1)*dx
     y(i) = cos(x)  ! fill with cosine
  end do

  call derivative (y,n,dx,dydx)  ! calculate dydx

  do i = 1,n  ! write result, -sin(x) and error
     x = (i-1)*dx
     print*,dydx(i),-sin(x),-sin(x)-dydx(i)
  end do

  deallocate(y,dydx)    ! finish

contains

  subroutine derivative (a,np,h,aprime) ! argument names different
    integer,intent(in) :: np            ! declare arguments
    real    ,intent(in) :: a(np),h
    real    ,intent(out):: aprime(np)
    integer             :: i            ! local variable

    do i = 1,np-1
       aprime(i) = (a(i+1)-a(i))/h   ! finite-difference formula
    end do
    aprime(np) = 0.

  end subroutine derivative

end program Deriv1
```

```fortran
program Deriv1
  implicit none
  integer             :: n,i
  real,allocatable:: y(:),dydx(:)
  real                :: x,dx

  write(*,'(a,$)') 'Input number of grid points:'; read*,n
  allocate (y(n),dydx(n))    ! allocate grid arrays

  dx = 10.0/(n-1)    ! grid spacing, assuming x from 0->10
  do i = 1,n
     x = (i-1)*dx
     y(i) = cos(x)  ! fill with cosine
  end do

  call derivative (y,n,dx,dydx)  ! calculate dydx

  do i = 1,n  ! write result, -sin(x) and error
     x = (i-1)*dx
     print*,dydx(i),-sin(x),-sin(x)-dydx(i)
  end do

  deallocate(y,dydx)     ! finish

contains
```

```fortran
contains

  subroutine derivative (a,np,h,aprime) ! argument names different
    integer,intent(in) :: np            ! declare arguments
    real   ,intent(in) :: a(np),h
    real   ,intent(out):: aprime(np)
    integer            :: i             ! local variable

    do i = 1,np-1
       aprime(i) = (a(i+1)-a(i))/h   ! finite-difference formula
    end do
    aprime(np) = 0.

  end subroutine derivative

end program Deriv1
```

Analysis

- Subroutine arguments can have different names from those in calling routine: what matters is order
- FD approximation becomes more accurate as grid spacing dx decreases
- Allocate argument arrays in the calling routine, *not* in the subroutine/function

Summary: first derivative

$$\frac{dy}{dx} \approx \frac{\Delta y}{\Delta x} = \frac{y_i - y_{i-1}}{x_i - x_{i-1}} = \frac{y_i - y_{i-1}}{h}$$

- Second derivative

$$\left(\frac{\partial^2 y}{\partial x^2} \right)_i = \frac{y_{i+1} - 2y_i + y_{i-1}}{h^2}$$

Exercise 3: Second derivative

- Write a subroutine that calculates the second derivative of an input 1D array, using the finite difference approximation
  - The inputs will be the array, number of points and grid spacing.
  - The resulting 1-D array can be an intent(out) argument.
  - The 2nd derivative will be calculated at i=2…n-1
  - Assume the derivative at the end points (i=1 and n) is 0.
- Test this routine by writing a main program that calls the subroutine with two idealized functions for which you know the correct answer, e.g., sin(x), x**2. Write out the your code's result, the correct result, and the error
- Hand in (to ETHFortran@gmail.com) your .f90 code and the results of your two tests