Programming and Modelling (week 38)

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Institute of Earth Sciences

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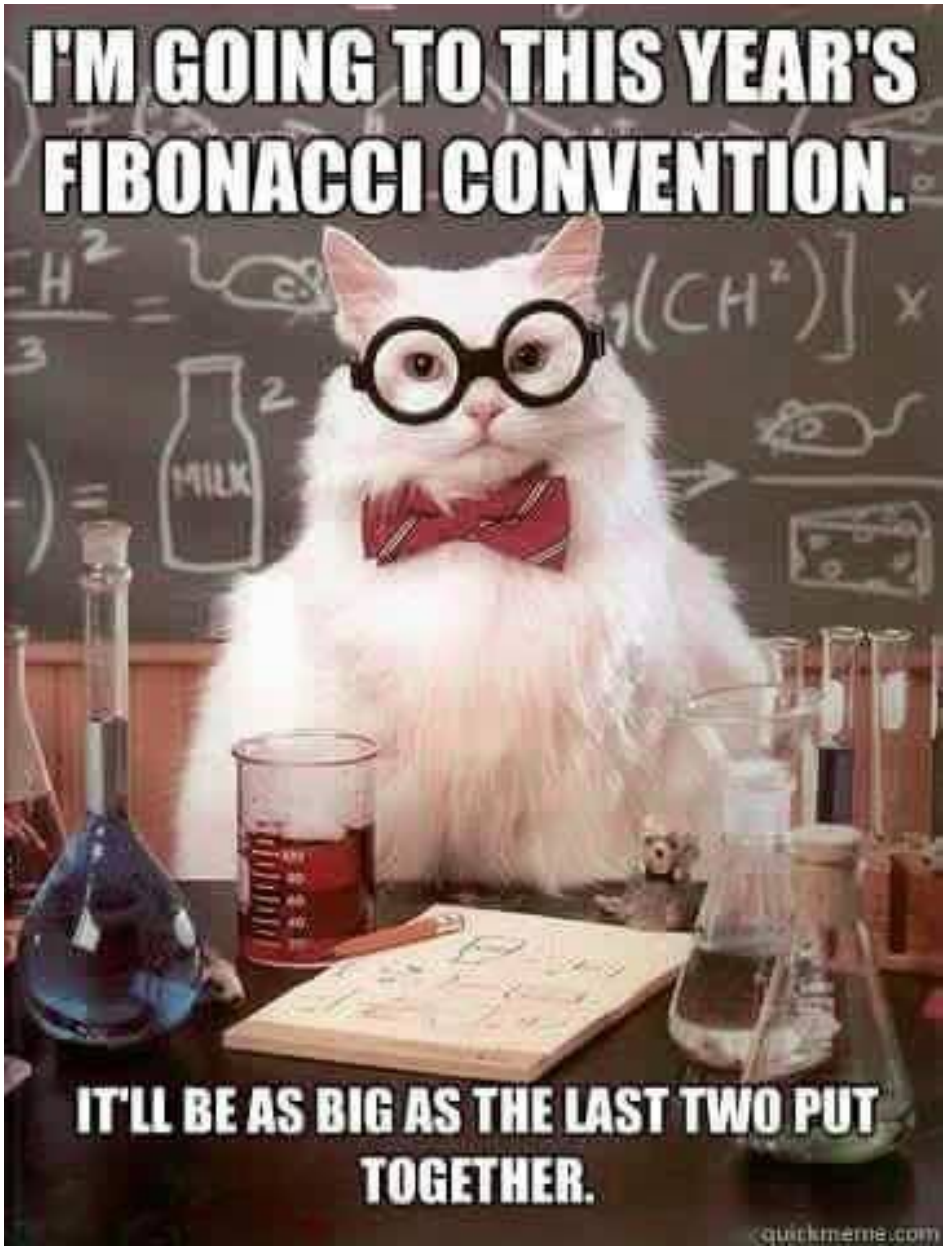
I'M GOING TO THIS YEAR'S FIBONACCI CONVENTION.
MILK
IT'LL BE AS BIG AS THE LAST TWO PUT TOGETHER.
quickmeme.com

Solve carefully...

230 – 220 x 0.5

You probably won't believe it, but the answer is 5!

feedback (1)

- a variable cannot have the same name as the program:

```
program factorial
implicit none

integer factorial
```

→ forbidden

- comments are placed before the instructions
- think about indentation

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- comments are placed before the instructions
- think about indentation
- when using `cos`, `sin`, etc ... do not declare them as real
- when declaring an array, its length must be a well defined constant, i.e. a NUMBER

feedback (2)

- equally share the typing/coding

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- equally share the typing/coding
- arrays in do-loops, do not forget `array(i)`
- do not write the whole array inside a do-loop
- you must know by heart the exact syntax of an `if` statement
- when dealing with real numbers, do not forget `1.`, `-7.`
- use keyboard more (shortcuts), use mouse less

feedback (3)

Methodology

- more preparation at home:

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  , then code
- write code progressively, compile and debug often !

function

- We have already seen intrinsic functions:
  cos, exp, log10, sin, ...
- Users can also define their own functions, such as for instance:
  - `convert_in_celsius(temp)`: takes a real temperature and returns its equivalent in Celsius degrees
  - `factorial(n)`: takes an integer number *n* and returns *n*
  - `compute_average(n,array)`: takes a real array of size n and returns its average

The factorial function (1)

Previously:

```
program factorial
implicit none

integer :: fact
integer :: i,n

write(6,*) 'enter a number'
read(5,*) n

if (n>0 .and. n<13) then

   fact=1
   do i=1,n
      fact=fact*i
      write(6,*) i,'! =',fact
   end do

else

   write(6,*) 'the input value of n'
   write(6,*) 'is not correct. Aborting.'

end if

end program
```

The factorial function (2)

```
program example
implicit none
integer, external :: factorial

print *,'fact  3',factorial(3)
print *,'fact  5',factorial(5)
print *,'fact  7',factorial(7)
print *,'fact 11',factorial(11)
print *,'fact 17',factorial(17)

end program

!=======================

function factorial(n)
implicit none
integer :: factorial,n

factorial=1
do i=1,n
   factorial=factorial*i
end do

end function

!=======================
```

```
thebeast:progmod geogarfield$ ./a.out
 fact  3           6
 fact  5         120
 fact  7        5040
 fact 11    39916800
 fact 17  -288522240
```

the compute_average function

```
program example
implicit none
integer, parameter :: n=100
real, dimension(n) :: tab
real, external     :: average

call random_number(tab)

write(*,*) 'avrg of tab is',average(n,tab)

call random_number(tab)

write(*,*) 'avrg of tab is',average(n,tab)

end program

!================================

function average(ntab,tab)
implicit none
integer :: ntab
real :: average,
real, dimension(ntab) ::tab

average=sum(tab)/real(ntab)

end function

!================================
```

```
thebeast:progmod geogarfield$ ./a.out
 avrg of tab is  0.53604215
 avrg of tab is  0.51591498
```

Using functions

The following uses function `factorial(n)` to compute the combinatorial coefficient

$$C(m,n) = \frac{m!}{n!(m-n)!}$$

where m and n are actual arguments:

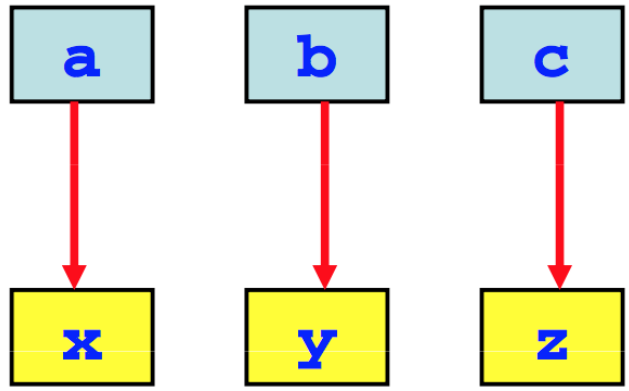
```
...
...
Cmn = factorial(m)/(factorial(n)*factorial(m-n))
...
```

Argument Association (1)

```
WRITE(*,*) Sum(a,b,c)



INTEGER FUNCTION Sum(x,y,z)
    IMPLICIT NONE
    INTEGER,INTENT(IN)::x,y,z
        ……..
END FUNCTION   Sum
```

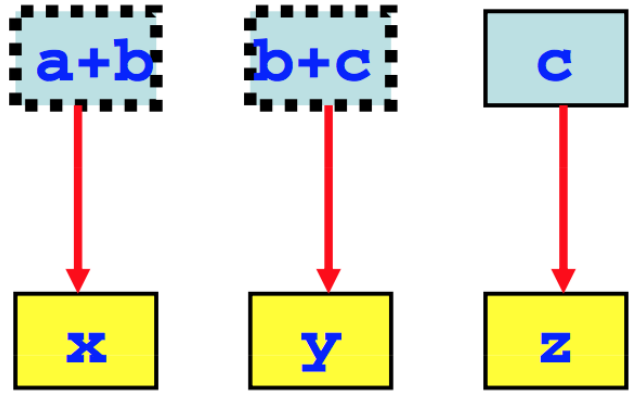


Argument Association (2)

```
WRITE(*,*) Sum(a+b,b+c,c)



INTEGER FUNCTION Sum(x,y,z)
    IMPLICIT NONE
    INTEGER,INTENT(IN)::x,y,z
        ……..
END FUNCTION   Sum
```

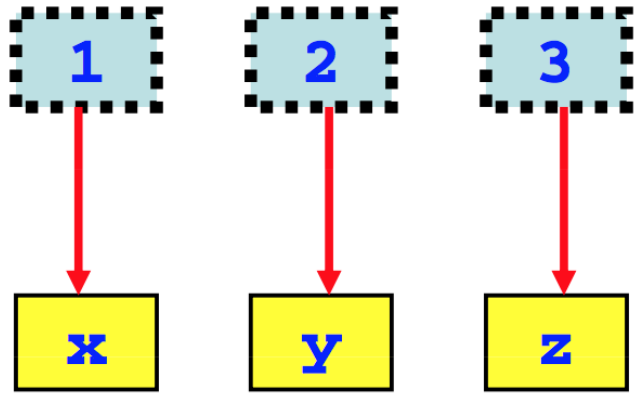


Argument Association (3)

```
WRITE(*,*) Sum(1, 2, 3)



INTEGER FUNCTION Sum(x,y,z)
    IMPLICIT NONE
    INTEGER,INTENT(IN)::x,y,z
        ……..
END FUNCTION   Sum
```



function vs subroutine

A function

- returns a value (or an array of values)
- has a type (integer, real, ...)
- is usually rather simple/short
- does not modify its arguments
- does not contain write statements

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A **subroutine**

- performs one or many tasks
- does not have a type
- is invoked with `call`
- has arguments (or not) and can return them modified

A very simple subroutine

```
program example
implicit none

call say_hello()

end program

!====================

subroutine say_hello()
implicit none

write(*,*) 'hello world !'

end subroutine

!====================
```

```
> ./a.out
hello world !
```

Example (2)

```
program example
implicit none

real :: vx,vy,vz,vel

call random_number(vx)
call random_number(vy)
call random_number(vz)

call compute_velnorm(vx,vy,vz,vel)

write(*,*) 'vect is    ',vx,vy,vz
write(*,*) 'its norm is',vel

end program

!====================

subroutine compute_velnorm(vect_x,vect_y,vect_z,vectnorm)
implicit none
real :: vect_x,vect_y,vect_z
real :: vectnorm

vectnorm=sqrt(vect_x**2+vect_y**2+vect_z**2)

end subroutine

!====================
```

```
> ./a.out
vect is 0.99755955 0.56682467 0.96591532
its norm is 1.4998026
```

Example (3)

```
program subdem
implicit none
real :: a,b,c,summ,sumsq

call INPUT(a,b,c)
call CALC(a,b,c,summ,sumsq)
call OUTPUT(summ,sumsq)

end program

!==================================

subroutine INPUT(x,y,z)
implicit none
real :: x,y,z
write(*,*) 'ENTER THREE NUMBERS: '
read *,x,y,z
end subroutine

!==================================

subroutine CALC(a,b,c,summ,sumsq)
implicit none
real :: a,b,c,summ,sumsq
summ  = a+b+c
sumsq = summ **2
end subroutine

!==================================

subroutine OUTPUT(summ,sumsq)
implicit none
real :: summ, sumsq
write(*,*) 'The sum of the numbers you entered are: ',summ
write(*,*) 'And the square of the sum is:',sumsq
end subroutine

!==================================
```

2D geometry (1)

- define three random points in $[0, 1] \times [0, 1]$
- compute the coordinates of the barycenter
- compute the area of the triangle they form with

$$A = \frac{1}{4}\sqrt{(a+b+c)(a+b-c)(a+c-b)(b+c-a)}$$

- compute the shortest side length of the triangle
- compute the angle values with

$$\cos\theta_A = \frac{\boldsymbol{AB} \cdot \boldsymbol{AC}}{|\boldsymbol{AB}|\,|\boldsymbol{AC}|}$$

2D geometry (2)

```
program example
implicit none
real, dimension(2) :: ptA,ptB,ptC,bary
real :: area
real :: Aangle,Bangle,Cangle
character(len=2) :: shortest

call random_number(ptA)
call random_number(ptB)
call random_number(ptC)

call barycenter(ptA,ptB,ptC,bary)

call area_triangle(ptA,ptB,ptC,area)

call find_shortest(ptA,ptB,ptC,shortest)

call compute_angles(ptA,ptB,ptC,Aangle,Bangle,Cangle)

write(*,*) '-----------------------------------'
write(*,*) 'pt A:',ptA
write(*,*) 'pt B:',ptB
write(*,*) 'pt C:',ptC
write(*,*) 'barycenter coordinates are ',bary
write(*,*) 'area of the triangle ', area
write(*,*) 'shortest side is ', shortest
write(*,*) 'angles        ', Aangle,Bangle,Cangle
write(*,*) 'sum of angles ', Aangle+Bangle+Cangle
write(*,*) '-----------------------------------'

end program
```

2D geometry (2)

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real, dimension(2) :: ptA,ptB,ptC,bary
real :: area
real :: Aangle,Bangle,Cangle
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call area_triangle(ptA,ptB,ptC,area)

call find_shortest(ptA,ptB,ptC,shortest)

call compute_angles(ptA,ptB,ptC,Aangle,Bangle,Cangle)

write(*,*) '-----------------------------------'
write(*,*) 'pt A:',ptA
write(*,*) 'pt B:',ptB
write(*,*) 'pt C:',ptC
write(*,*) 'barycenter coordinates are ',bary
write(*,*) 'area of the triangle ', area
write(*,*) 'shortest side is ', shortest
write(*,*) 'angles        ', Aangle,Bangle,Cangle
write(*,*) 'sum of angles ', Aangle+Bangle+Cangle
write(*,*) '-----------------------------------'

end program
```

```
subroutine barycenter(ptA,ptB,ptC,bary)
implicit none
real, dimension(2) :: ptA,ptB,ptC,bary

bary(1)=(ptA(1)+ptB(1)+ptC(1))/3.
bary(2)=(ptA(2)+ptB(2)+ptC(2))/3.

end subroutine

!==========================

subroutine area_triangle(ptA,ptB,ptC,area)
implicit none
real, dimension(2) :: ptA,ptB,ptC
real :: AB,BC,AC,area

AB=sqrt( (ptB(1)-ptA(1))**2 + (ptB(2)-ptA(2))**2 )
BC=sqrt( (ptB(1)-ptC(1))**2 + (ptB(2)-ptC(2))**2 )
AC=sqrt( (ptA(1)-ptC(1))**2 + (ptA(2)-ptC(2))**2 )

area=0.25*sqrt((AB+BC+AC)*(AC+AB-BC)*(AB+BC-AC)*(BC+AC-AB))

end subroutine

!==========================

subroutine find_shortest(ptA,ptB,ptC,shortest)
implicit none
real, dimension(2) :: ptA,ptB,ptC
real :: AB,BC,AC
character(len=2) :: shortest

AB=sqrt( (ptB(1)-ptA(1))**2 + (ptB(2)-ptA(2))**2 )
BC=sqrt( (ptB(1)-ptC(1))**2 + (ptB(2)-ptC(2))**2 )
AC=sqrt( (ptA(1)-ptC(1))**2 + (ptA(2)-ptC(2))**2 )

if (AB<AC .and. AB<BC) shortest='AB'
if (AC<AB .and. AC<BC) shortest='AC'
if (BC<AB .and. BC<AC) shortest='BC'

end subroutine
```

2D geometry (3)

```
program example
implicit none
real, dimension(2) :: ptA,ptB,ptC,bary
real :: area
real :: Aangle,Bangle,Cangle
character(len=2) :: shortest

call random_number(ptA)
call random_number(ptB)
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call compute_angles(ptA,ptB,ptC,Aangle,Bangle,Cangle)

write(*,*) '-----------------------------------'
write(*,*) 'pt A:',ptA
write(*,*) 'pt B:',ptB
write(*,*) 'pt C:',ptC
write(*,*) 'barycenter coordinates are ',bary
write(*,*) 'area of the triangle ', area
write(*,*) 'shortest side is ', shortest
write(*,*) 'angles        ', Aangle,Bangle,Cangle
write(*,*) 'sum of angles ', Aangle+Bangle+Cangle
write(*,*) '-----------------------------------'

end program
```

$$\cos\theta_A = \frac{\boldsymbol{AB}\cdot\boldsymbol{AC}}{|\boldsymbol{AB}|\,|\boldsymbol{AC}|}$$

```
subroutine compute_angles(ptA,ptB,ptC,Aangle,Bangle,Cangle)
implicit none
real, dimension(2) :: ptA,ptB,ptC
real :: Aangle,Bangle,Cangle
real :: AB,BC,AC,dot_pr,pi

pi=4.*atan(1.)

AB=sqrt( (ptB(1)-ptA(1))**2 + (ptB(2)-ptA(2))**2 )
BC=sqrt( (ptB(1)-ptC(1))**2 + (ptB(2)-ptC(2))**2 )
AC=sqrt( (ptA(1)-ptC(1))**2 + (ptA(2)-ptC(2))**2 )

dot_pr=(ptB(1)-ptA(1))*(ptC(1)-ptA(1)) &
      +(ptB(2)-ptA(2))*(ptC(2)-ptA(2))

Aangle=acos(dot_pr/AB/AC)/pi*180.

dot_pr=(ptA(1)-ptB(1))*(ptC(1)-ptB(1)) &
      +(ptA(2)-ptB(2))*(ptC(2)-ptB(2))

Bangle=acos(dot_pr/AB/BC)/pi*180.

dot_pr=(ptA(1)-ptC(1))*(ptB(1)-ptC(1)) &
      +(ptA(2)-ptC(2))*(ptB(2)-ptC(2))

Cangle=acos(dot_pr/AC/BC)/pi*180.

end subroutine
```

2D geometry (4)

```
program example
implicit none
real, dimension(2) :: ptA,ptB,ptC,bary
real :: area
real :: Aangle,Bangle,Cangle
character(len=2) :: shortest

call random_number(ptA)
call random_number(ptB)
call random_number(ptC)

call barycenter(ptA,ptB,ptC,bary)

call area_triangle(ptA,ptB,ptC,area)

call find_shortest(ptA,ptB,ptC,shortest)

call compute_angles(ptA,ptB,ptC,Aangle,Bangle,Cangle)

write(*,*) '-----------------------------------'
write(*,*) 'pt A:',ptA
write(*,*) 'pt B:',ptB
write(*,*) 'pt C:',ptC
write(*,*) 'barycenter coordinates are ',bary
write(*,*) 'area of the triangle ', area
write(*,*) 'shortest side is ', shortest
write(*,*) 'angles        ', Aangle,Bangle,Cangle
write(*,*) 'sum of angles ', Aangle+Bangle+Cangle
write(*,*) '-----------------------------------'

end program
```

```
thebeast:progmod geogarfield$ ./a.out
 -----------------------------------
 pt A:  0.99755955      0.56682467
 pt B:  0.96591532      0.74792767
 pt C:  0.36739087      0.48063689
 barycenter coordinates are   0.77695531      0.59846306
 area of the triangle   5.84263988E-02
 shortest side is AB
 angles           87.876724       75.846550       16.276726
 sum of angles    180.00000
 -----------------------------------
```

```
program elefant

use structures

implicit none

include 'mpif.h'

CALL mpi_init(ierr)
call mpi_comm_size (mpi_comm_world,nproc,ierr)
call mpi_comm_rank (mpi_comm_world,iproc,ierr)

!==================================!
                                   !
call header                        !
call clean                         !
call open_files                    !
call read_n_compute_parameters     !
call write_parameters              !
call cailloux_setup                !
call read_materials                !
call grid_setup                    !
call cloud_setup                   !
call timevisu_setup                !
call tracers_setup                 !
call vgrid_setup                   !
call stretch                       !
call landscape_setup               !
call lsurface_setup                !
call paint_stripes                 !
call material_layout               !
call strain_history                !
call nu_layout                     !
call temperature_layout            !
call initialise_mumps_V            !
call initialise_mumps_T            !
call initialise_mumps_P            !
call matrix_setup                  !
call compute_tot_volume_and_mass   !
call compute_elsize                !
call compute_element_centers       !
call compute_hydr_pressure         !
call compute_qcoords               !
                                   !
do istep=1,nstep !---------------------------- timestepping
                                             !
   iter=0                                    !
   conv=.false.                              !
                                             !
   do while (.not.conv .and. iter<abs(niter))!-----
                                             !
      iter=iter+1                            !
                                             !
```