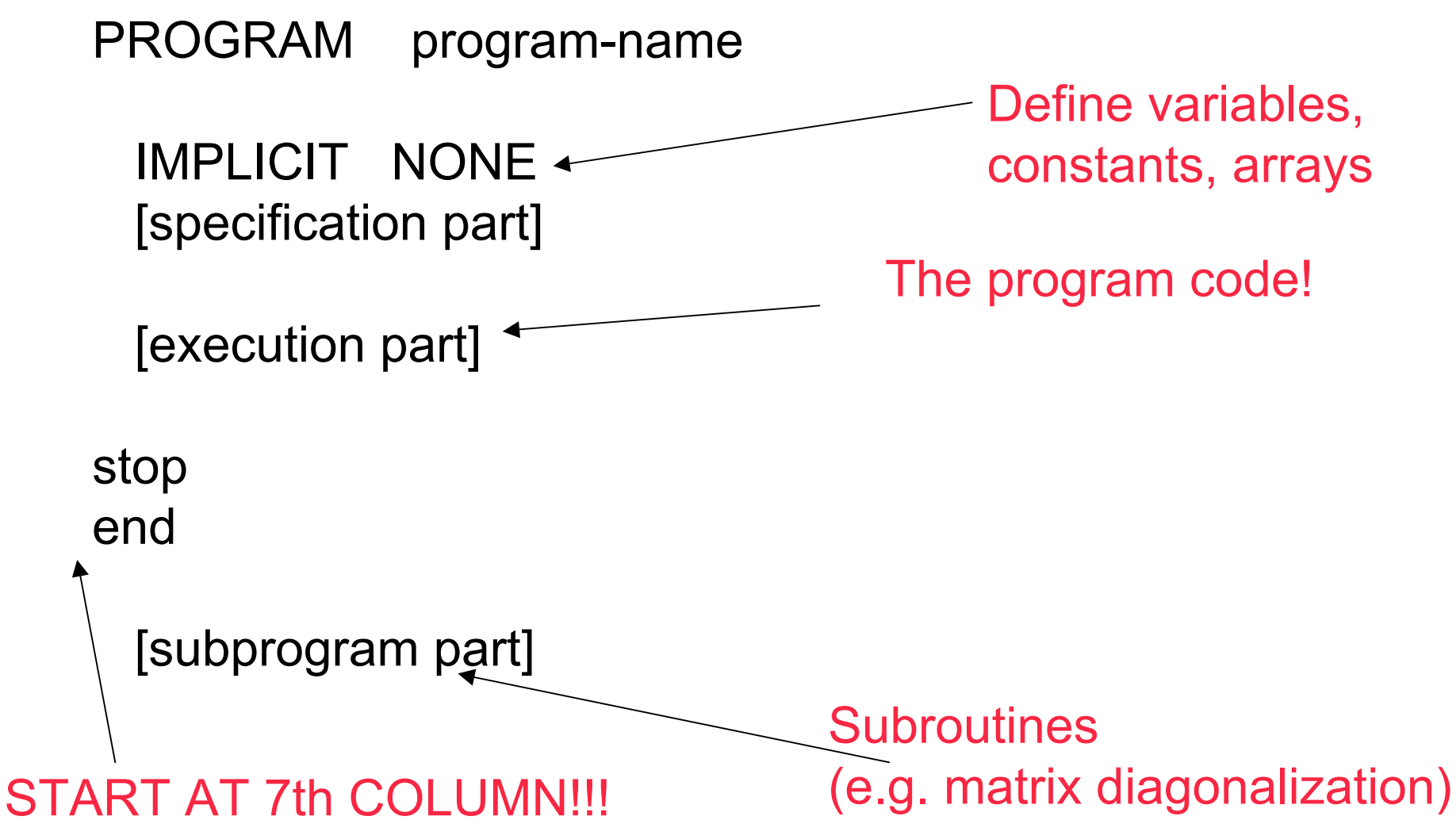
I. Basics of F90/F77 programming



Specification part-- variables

* INTEGER : the variables in list can hold integers
* REAL: the variables in list can hold real numbers
* COMPLEX: the variables in list can hold complex numbers
* LOGICAL: the variables in list can hold logical values
  (i.e., true or false)
* CHARACTER: the variables in list can hold character strings

Examples:

```
integer  I, j, n, ntotal, naverage
double precision Hamil, Q, Energy, Z
character(2)  Element
```

Specification part-- variable arrays

Examples:

```
double precision a(10), b(10), c(10)
double precision H(10,10)
```

In this example, everything is declared as real variables.
Each of a, b, and c are one-dimensional arrays of length 10.
In contrast, H is a two-dimensional array which is 10x10.

In other words, a, b, and c are like vectors, and H is a matrix!

Parameter statements

- Not really parameters, but instead constants
- Can be integer, real, etc.
- Should declare variables as real, integer, etc. before parameter statement

```
PARAMETER  pi=3.141592
PARAMETER  MAX=100
```

Once set, parameters cannot be changed within your code!

Comments

- Comments start with c
- No function other than notes for programmer
- Still important!

```
c Program to compute eigenfunctions and eigenvalues
c for a particle in a one-dimensional potential
```

Comments are especially important for anyone else who inherits your code!

Program layout-- execution part

```
PROGRAM    program-name

   IMPLICIT   NONE
   [specification part]

   [execution part]

Stop
end

   [subprogram part]
```

The execution part is control statements, subroutine calls, functions, and intrinsic functions

If/then/else

- Control statement
- Can nest as many as one needs

Just a single if statement… no then or else:

```
if (x<0) x=0
```

…alternately, if(x.lt.0) x=0

Or, when several conditions are desired:

```
if (x<0) then
  x=0
else
  if (x>100) x=100
endif
```

Notice indentation!

Terminate with “endif”

Do loops…

- Another control statement
- Useful for repeated calculations

```
INTEGER  n
REAL  x,y,pi

pi=4.0d0*atan(1.0)

do n=1,100
  x=pi*n
  y=cos(x)
  write(6,*) n,y
enddo
```

Integer n takes on Values 1,2,3,…,100

Again indentation

Terminate do loop

Goto statements

- Often best to avoid as much as possible
- Very often used in conjunction with “if” statements

```
      REAL  x

            if (x<0) goto 100

               …

100      x=0
```

Statements that
Are only done if x>0

Line number 100 (just a tag or label). Start in first column!

Intrinsic functions

- Mathematical functions
- Intrinsic to f90 compiler

```
real x,y

y=cos(x)
y=exp(x)
y=atan(x)
```

Cosine of argument x

$y=e^x$

$y=\tan^{-1}(x)$

Links to intrinsic function list given in my webpage

Input/output

- Input data usually from “read” statement… Input file
- Output results from “write” statement… screen or output file
- Everything needs a unit number
- Format statements… useful, sometimes needed, can be a pain

```
INTEGER  n,i,j,k
REAL  x,y,z

open(unit=10,file='input.dat')
open(unit=11,file='output.dat')

read(10,*) i,j,k,x,y
n=I+j+k
z=x+y
write(11,*) n,z
write(6,*) n,z
```

Unformatted input and output

unit=6 reserved for output to screen

For the first project…

```
c Simulation of radioactive decay

      program decay
C declare variables/arrays (specification part)
      implicit none
      double precision n_uranium(100), t(100),tau,dt
      integer n

      call initialize(n_uranium,t,tau,dt,n)
      call calculate(n_uranium,t,tau,dt,n)
      call store(n_uranium,t,n)

      stop
      end
```

Initialize subroutine

```
subroutine initialize(nuclei,t,tc,dt,n)
double precision nuclei(100),t(100),tc,dt,time
integer n
print *,'initial number of nuclei '
read(5,*) nuclei(1)
print *,'time constant'
read(5,*) tc
print *,'time step'
read(5,*) dt
print *,'total time'
read(5,*) time
t(1)=0.0d0
n=min(int(time/dt),100)
return
end
```

Calculate subroutine

```
subroutine calculate(n_uranium,t,tau,dt,n)
implicit none
double precision n_uranium(n),t(n),tau,dt
integer n,i
do i=1,n-1
        n_uranium(i+1) = n_uranium(I)*(1.0d0-dt/tau)
        t(i+1) = t(I)+dt
return
end
```

Store subroutine

```
      subroutine store(n_uranium,t,n)
      double precision n_uranium(n),t(n)
      integer i,n
      open(unit=1,file='decay.dat')
       do i=1,n
              write(1,20) t(i),n_uranium(i)
       enddo
20    format(1x,1p,2(f12.5,2x)
      return
      end
```