CEE 618 Scientific Parallel Computing (Lecture 6): Object Oriented Programming (OOP) of FORTRAN 2003 and OpenMP vs. MPI

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ssh fractal - ssh c18.

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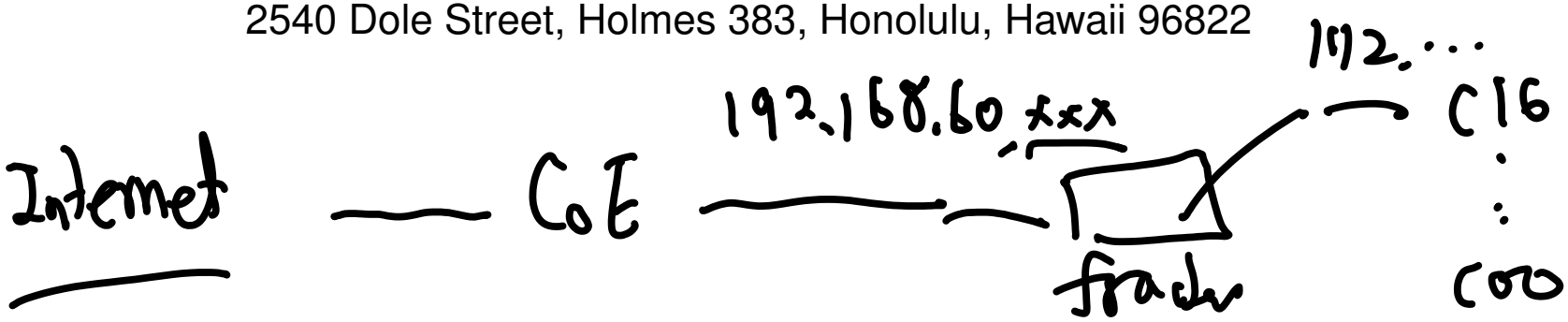


Table of Contents

Outline

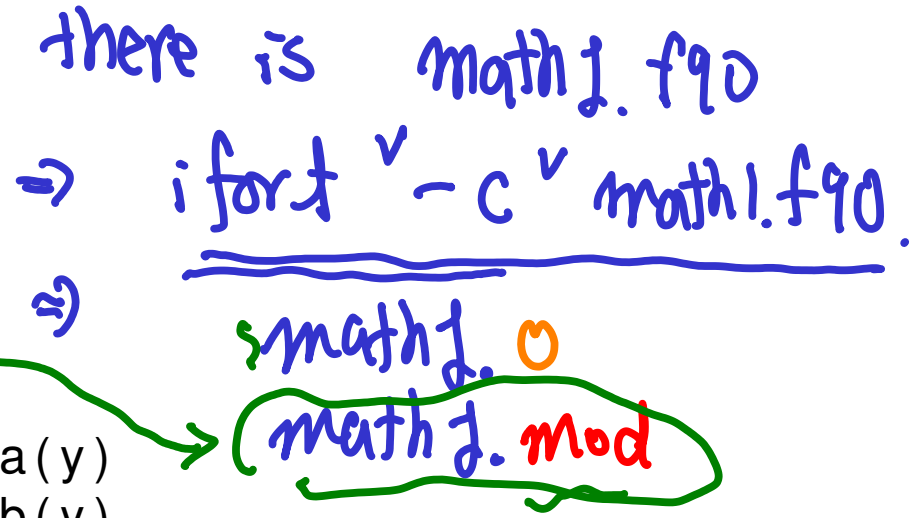
Data type, customized

```
1  module mytype
2     implicit none
3     type person
4        character (len=20) :: pname
5        integer    (kind=8) :: age
6        character (len=14) :: phone(2)
7     end type person
8  end module
9
10 program typetest
11    use mytype
12    implicit none
13    type(person) :: me(2)
14    me(1)%pname="Albert␣S.␣Kim"    ;   me(1)%age=32
15    me(1)%phone(1)="1-808-956-3718"
16    me(1)%phone(2)="1-808-233-9491"
17     write(*,"(A20)") me(1)%pname
18     write(*,"(I2)" ) me(1)%age
19     write(*,"(A14)") me(1)%phone(1)
20     write(*,"(A14)") me(1)%phone(2)
21 end
```

Screen outputs

```
./mytype.x
Albert S. Kim
32
1-808-956-3718
1-808-233-9491
```

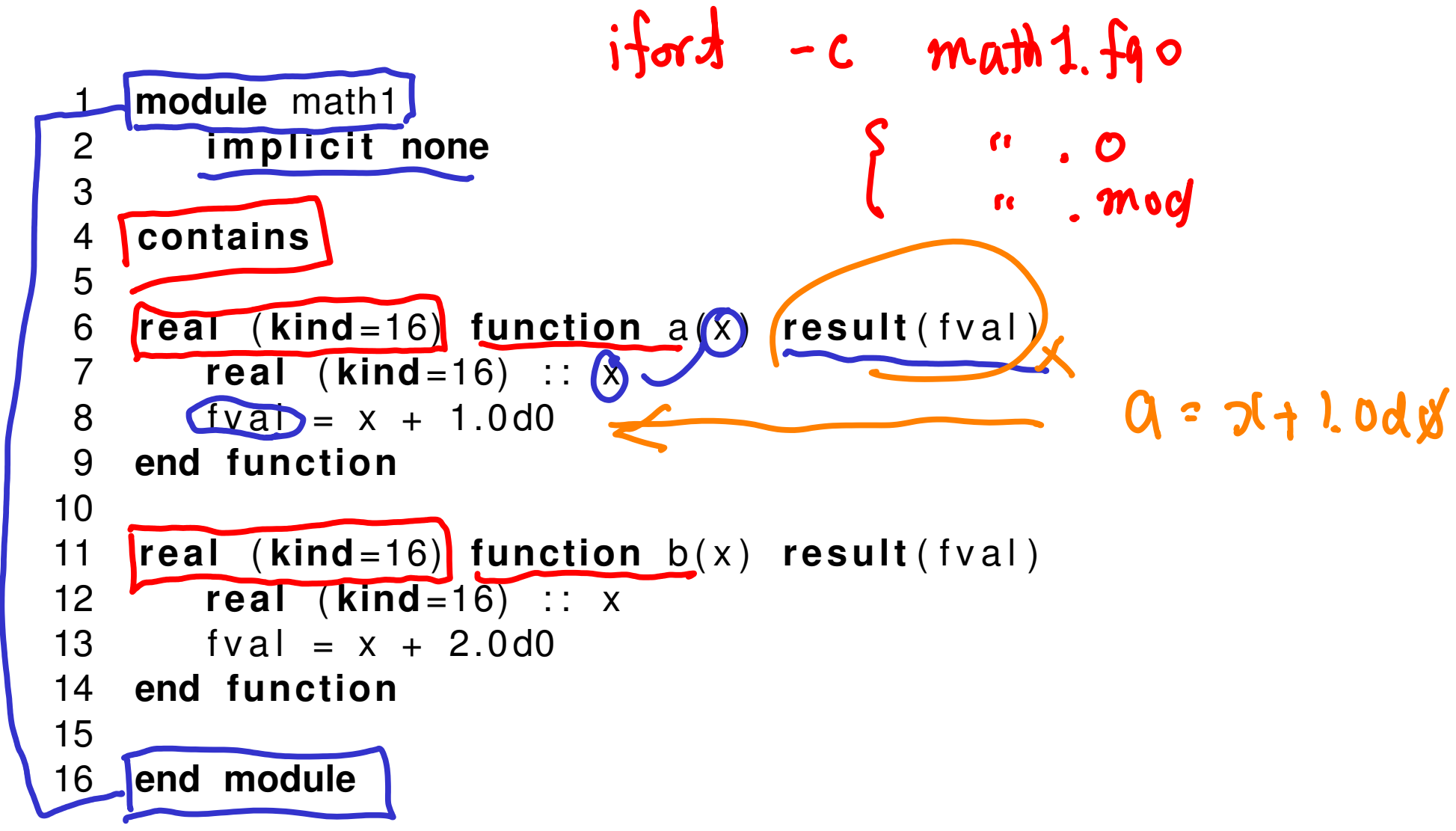
Main program 1 (main1.f90)




```
1   program main1
2   use math1
3   implicit none
4   real (kind=16) :: y = 2.0d0
5   write(*,"(2(2x,e22.15))") y, a(y)
6   write(*,"(2(2x,e22.15))") y, b(y)
7   end program
```

```
./main1.x
0.20000000000000E+01 0.30000000000000E+01
0.20000000000000E+01 0.40000000000000E+01
```

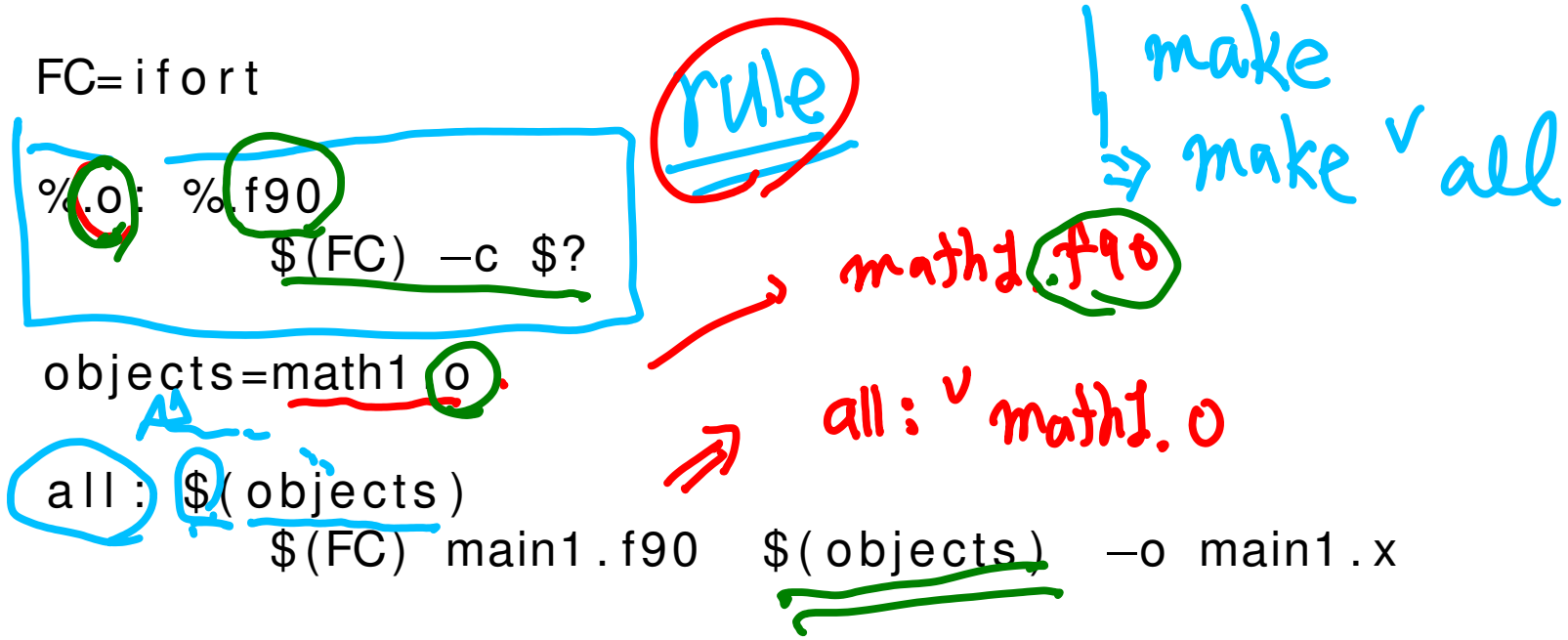
math1 module file (math1.f90)




```
 1  module math1
 2      implicit none
 3
 4  contains
 5
 6  real (kind=16) function a(x) result(fval)
 7      real (kind=16) :: x
 8      fval = x + 1.0d0
 9  end function
10
11  real (kind=16) function b(x) result(fval)
12      real (kind=16) :: x
13      fval = x + 2.0d0
14  end function
15
16  end module
```

Makefile

```
1  FC=ifort
2
3  %.o: %.f90
4          $(FC) -c $?
5
6  objects=math1.o
7
8  all: $(objects)
9          $(FC) main1.f90 $(objects) -o main1.x
10
11 run:
12         ./main1.x
13 clean:
14         rm -f *.o *.x *.mod
```



- “make” command will show (afer “make clean”)

```
$ ifort -c math1.f90
$ ifort main1.f90 math1.o -o main1.x
```

Main program 2 (main2.f90)

```
 1  program main
 2  use math1
 3  use math2
 4  implicit none
 5  real (kind=16) :: y = 2.0d0
 6  write(*,"(2(2x,e22.15))") y, a(y)
 7  write(*,"(2(2x,e22.15))") y, b(y)
 8  write(*,"(2(2x,e22.15))")
 9  write(*,"(10(2x,f16.9))") y, a2(y),  b2(y), b3(y), b4(y)
10  end program
```

./main2.x

0.200000000000000E+01 0.300000000000000E+01

0.200000000000000E+01 0.400000000000000E+01

2.000000000 3.000000000 4.000000000 4.000000000 4.000000000

math2 module file (math2.f90)

```
 1  module math2
 2      implicit none
 3  contains
 4  real (kind=16) function a2(x) result(fval)
 5      real (kind=16) :: x
 6      fval = x + 1.0d0
 7  end function
 8  real (kind=16) function b2(x) result(fval)
 9      real (kind=16) :: x
10      fval = x + 2.0d0
11  end function
12
13  real (kind=16) function b3(x) result(fval)
14      real (kind=16) :: x
15      fval = a2(x) + 1.0d0
16  end function
17  real (kind=16) function b4(x) result(fval)
18      use math1, only : a
19      real (kind=16) :: x
20      fval = a(x) + 1.0d0
21  end function
22  end module
```

// a(x) in math1.f90

// b(x) in math1.f90

⇒ fval = x + 2.0d0

math1 module file (math1.f90)

Again ...

```
 1  module math1
 2      implicit none
 3
 4  contains
 5
 6  real (kind=16) function a(x) result(fval)
 7      real (kind=16) :: x
 8      fval = x + 1.0d0
 9  end function
10
11  real (kind=16) function b(x) result(fval)
12      real (kind=16) :: x
13      fval = x + 2.0d0
14  end function
15
16  end module
```

Makefile

```
1  FC=ifort
2  %.o: %.f90
3          $(FC) -c $?
4  objects=math1.o     math2.o
5
6  all: $(objects)
7          $(FC) main2.f90  $(objects)  -o main2.x
8
9  run:
10          ./main2.x
11 clean:
12         rm -f *.o *.x *.mod
```

- “make” command will show (afer “make clean”)

```
$ ifort␣-c␣math1.f90
$ ifort␣-c␣math2.f90
$ ifort␣main1.f90␣math1.o␣math2.o␣-o␣main1.x
```

Main program 2 (main2.f90)

```
use physics
implicit none
write(*,"('␣Pi␣value␣is␣',1x,F22.15)")   pi
write(*,"('␣Avogadro␣number␣is␣',1x,e22.15)") Na
write(*,"('␣Gas␣constant␣␣is␣',1x,e22.15)")    Rg_J_MolKlvn
write(*,"('␣Boltzmann␣constant␣is␣',1x,e22.15)") KBoltzman
end
```

physics module file (physics.f90) and screen output

```
module physics
implicit none
real (kind=16), parameter :: pi=3.14159265358979323846D0
real (kind=16), parameter :: Na=6.02214129d23 ! per mole
real (kind=16), parameter :: Rg=8.3144621 ! J / mol K
real (kind=16), parameter :: Rg_J_MolKlvn = Rg
real (kind=16), parameter :: Rg_kJ_MolKlvn=8.3144621D-3 ! J/mol K
real (kind=16), parameter :: KBoltzman = 1.3806488d-23 ! Joule/K
end module
```

- Screen output by “make” followed by “make run”

Pi value is 3.141592653589793

Avogadro number is 0.602214129000000E+24

Gas constant in [J/ mol K] is 0.831446170806885E+01

Boltzmann constant is 0.138064880000000E-22

Outline

opi4.f90

```
program main
use omp_lib
double precision  PI25DT
parameter         (PI25DT = 3.14159265358979323846264 3d0)
double precision  pi, h, sum, x, f, a,  time, T1, T2
integer           n,i
f(a) = 4.d0 / (1.d0 + a*a)
n = 1250000000
h = 1.0d0/dble(n)
sum  = 0.0d0
T1 = TIME()
!$omp parallel do private (i,x) reduction (+:sum)
do i = 1, n
    x = h * (dble(i) - 0.5d0)
    sum = sum + f(x)
enddo
pi = h * sum
T2 = TIME()
write(*, *) pi, abs(pi - PI25DT)
stop
end
```

MPI_REDUCE

MPI_SUM

do i = myid+1, n, numprocs

Compile and Run

- Compile

  $ ifort -openmp opi4.f90 -o opi4.x

- Determine the number of threads. Try 1, 2, 4, 6, and 8

  $ export OMP_NUM_THREADS=8

- Execution is identical to serial cases. Measure thr running time.

  $ time ./opi4.x

opi7.f90

```
 program main
 use omp_lib
 double precision  PI25DT
 parameter         (PI25DT = 3.14159265358979323846264 3d0)
 double precision  pi, h, sum, x, f, a, T1, T2, time
 integer n, myid, numthreads,   i
 f(a) = 4.d0 / (1.d0 + a*a)
 n=1250000000  ; h=1.0d0/dble(n) ; sum=0.0d0 ; T1=TIME()
!$OMP PARALLEL private (myid)
 myid       = OMP_GET_THREAD_NUM()
 numthreads = omp_get_num_threads()
 write(*,*) myid, numthreads
!$OMP  DO SCHEDULE(STATIC, numthreads) reduction(+:sum)
 do i = 1, n
    x = h * (dble(i) - 0.5d0)
    sum = sum + f(x)
 enddo
!$OMP end do
!$OMP END PARALLEL
 pi = h * sum ; T2 = TIME()  ; write(*, *) pi, abs(pi - PI25DT)
stop
```

opi3.f90

```
program main
use omp_lib
double precision  PI25DT
parameter        (PI25DT = 3.14159265358979323846264 3d0)
double precision  pi, h, sum, x, f, a, T1, T2, time
integer n, i
f(a) = 4.d0 / (1.d0 + a*a)
n=1250000000       ;  h = 1.0d0/dble(n) ; sum  = 0.0d0
T1 = TIME()
!$omp parallel private (i,x)
!$omp do reduction (+:sum)
do i = 1, n
    x = h * (dble(i) - 0.5d0)
    sum = sum + f(x)
enddo
!$omp end do
!$omp end parallel
pi = h * sum
T2 = TIME()
write(*, *) pi, abs(pi - PI25DT)
stop
```

Discussion

OpenMP

1. is relatively easy to learn in comparison to MPI, but the performance is not straightforward.
2. is better for small shared memory systems when 4-8 times speedup is remarkable.
3. is more sensitively depending on compilers and hardware.
4. does not communicate through network but channels through processors/cores.
5. is not the best for (very) large scale simulation with flexibility.
6. can be used toghether with MPI, called hybrid parallelization.