CEE 618 Scientific Parallel Computing (Lecture 2): FORTRAN, Library, Make, and PBS

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Outline

FORTRAN

- All the sample codes are located under /**opt/cee618s13/** from which you can copy files.
- I recommend you to generate the same directory structure under your $HOME directory.

```
$ mkdir cee618s13
$ cd cee618s13
$ mkdir class01
$ mkdir class02
```

- Then, store all files of the last class in 'class01' and today's files in 'class02'.

```
$ cd class02
$ cp -r /opt/cee618s13/class02/* ./
```

Summation code from 1 to 100, $\sum_{i=1}^{100} n$

```
1 program sum100
2 implicit none
3 integer :: i, n=100, nsum=0
4 do i = 1, n
5     nsum = nsum + i
6 enddo
7 print *, nsum
8 stop
9 end
```

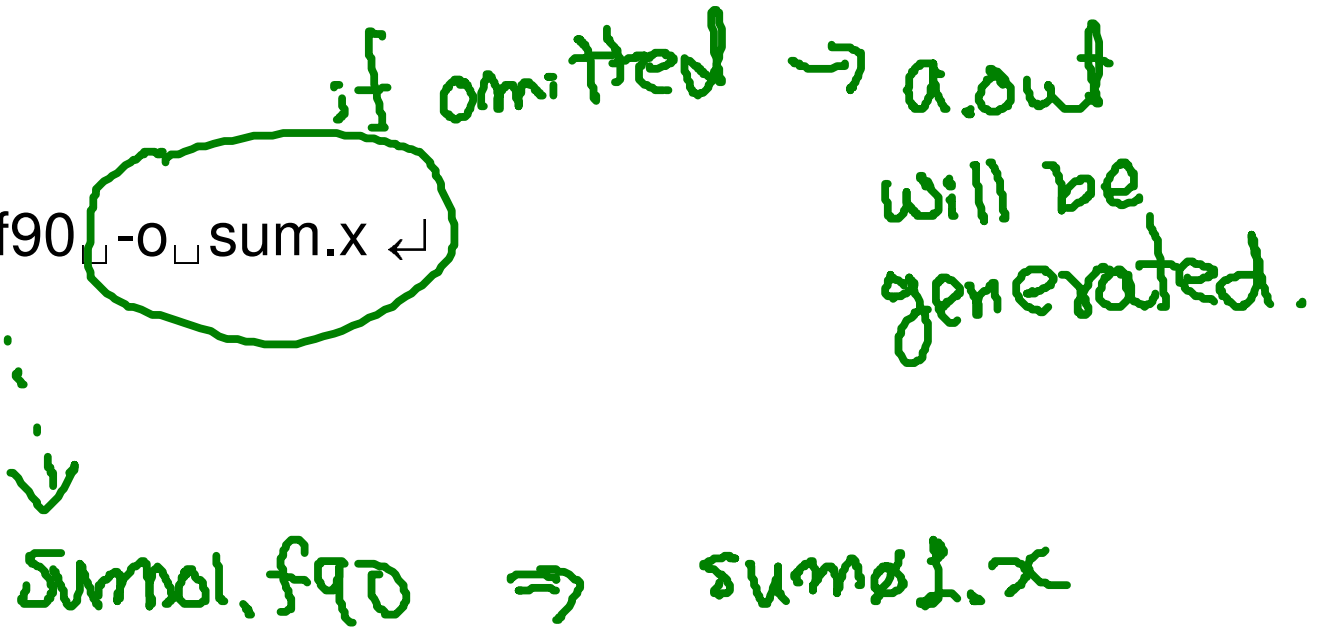
codes/sum/sum.f90

This code can be modified for your homework to calculate $\sum_{i=1}^{100} n^3$

How to compile and run

- $␣ifort␣sum.f90␣-o␣sum.x ↵
- $␣sum.x ↵

5050



Outline

Monty Hall Paradox

Suppose you're on a game show, and you're given the choice of three doors: Behind one door is a car; behind the others, goats. You pick a door, say No. 1, and the host, who knows what's behind the doors, opens another door, say No. 3, which has a goat. He then says to you, "Do you want to pick door No. 2?" Is it to your advantage to switch your choice?

Search "The Monty Hall Problem" in YouTube:
http://www.youtube.com/watch?v=mhlc7peGlGg

Possible Answers: What is your own answer?

1. Switch
2. Stay
3. No difference

Correct Answer: Switch

1. Reference: Chapter 1. "*Bias Monte Carlo Methods in Environmental Engineering*" in "Applications of Monte Carlo Methods in Biology, Medicine and Other Fields of Science" edited by Charles J. Mode, ISBN 978-953-307-427-6. Freely downloadable at `http://albertsk.org/publications/`
2. Test an example case.

Selecting Good Wines

(Answer)

- A wine box has 12 bottles, 3 of which contain spoiled wine. A sample of 4 bottles is randomly selected from the box. Find the probability that you don't selected any spoiled wine.

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(Answer)

$$p = \frac{C_0^3 C_4^9}{C_4^{12}} = \frac{1\,(126)}{495} = 0.254545 \tag{1}$$

where

$$C_k^N = \frac{N!}{k!\,(N-k)!} \tag{2}$$

The number of ways of picking k unordered outcomes from N possibilities. Read "N **choose** k."

Program

There are is a main program file, **wine.f90**, and two additional files, **selectn.f90**, and **spoiled.f90**, which of each contains one subroutine.

- nran: the number of wine bottles randomly selected, e.g., **4** out of **12**.
- nunspoiled: the number of events that spoiled wine bottles are not selected.
- ntotal: the total number of computer experiments.

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- nran: the number of wine bottles randomly selected, e.g., **4** out of **12**.
- nunspoiled: the number of events that spoiled wine bottles are not selected.
- ntotal: the total number of computer experiments.
- ID: the ID array of randomly selected bottles with "nran" elements. For example, if four bottles [2, 5, 7, and 10] contain spoiled wine, then ID(1)=**2**, ID(2)=**5**, ID(3)=**7**, and ID(4)=**10**.

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- wine: logical data
  1. If wine is "**.true.**", then none of "nran" bottles contains spoiled wine.
  2. If wine is "**.false.**", then at least one of "nran" bottles contains spoiled wine.
- Probability = the number of selecting "nran" unspoiled wine bottles divided by the total number of trial, i.e., **nunspoiled / ntotal**.

wine.f90

```
1  program wine_select
   implicit none
3  integer                 :: i, j, k, nunspoiled=0
   integer, parameter      :: nbottle=12,nspoiled=3, nran=4, ntotal
       =1000000
5  integer                 :: ID(nran)
   real                    :: probability
7  logical                 :: wine

9  do i = 1, ntotal
     call selectn(nbottle, nran, ID)
11   call spoiled(nspoiled,nran, ID, wine)
     if(wine == .true.) nunspoiled = nunspoiled + 1
13 enddo
   probability = DBLE(nunspoiled) / DBLE(ntotal)
15 write(*,"('Probability is',1X,F9.6 )") probability

17 stop
   end
```

selectn.f90

```
subroutine selectn(nbottle, nran, ID)
implicit none
integer :: nbottle, nran, ID(nran), i, j, jproduct
real    :: X
logical :: overlap
call random_number(X)
ID(1) = int( dble(nbottle) * X + 1.0 )
do i = 2, nran
  overlap=.true.
  do while (overlap==.true.)
    call random_number(X)
    ID(i) = int( dble(nbottle) * X + 1.0 ) ; jproduct = 1
    do j = 1, i-1
      jproduct = jproduct * (ID(j)-ID(i) )
    enddo
    if(jproduct/=0) overlap =.false.
  enddo
enddo
return
end
```

spoiled.f90

```
subroutine spoiled(nspoiled, nran, ID, wine)
implicit none
integer  :: i
integer  :: nspoiled,nran, ID(nran)
logical  :: wine
wine=.true.
do i = 1, nran
   if(ID(i) <= nspoiled) then
      wine = .false.
      exit
   endif
enddo
return
end
```

codes/wine/spoiled.f90

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  3. Subroutine selectn (nran, ID) calls intrinsic FORTRAN 90 subroutine **random_number (X)**, where $0 < X < 1.0$ is a random number.
  4. In total, 3 files = 1 man program + 2 subroutine files.
- Simple compilation
  1. ifort␣*.f90
  2. ifort␣wine.f90␣selectn.f90␣spoiled.f90 ⇒ a.out
  3. ifort␣wine.f90␣selectn.f90␣spoiled.f90␣-o␣wine.x
- In compilation 1 and 2, "**a.out**" is created as an executable file. And, in compilation 3, "wine.x" as specified.

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- Method 1: compile subroutine files individually and use them.
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  3. ifort wine.f90 selectn.**o** spoiled.**o** -o wine.x

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- All equivalent to: ifort wine.f90 selectn.f90 spoiled.f -o wine.x

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     - “ar” indicates **archive** with options “-r” to **replace** (also create if not present) and “-v” for **verbose**. In other words, the two subroutine files are contained in a newly generated library file “libwine.a”. Note that a library file should have extension “**.a**”.

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  4. (*alternatively but important*) ifort␣wine.f90␣**-L./**␣-**lwine**␣-o␣wine.x
     - “-L” indicates that what follows is a library path, which is in this case the current directory “./”. “-l” means library file of extension “.a” with partial name “wine” after “lib”, i.e., “lib**wine**.a”

Outline

“Make utility”

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   This will update objects files whose source codes are **younger**.
5. If you prepared a Makefile as “Makefile.2”, use “-f” option:

   $␣**make␣-f ␣Makefile.2**

Makefile

```
all:
	ifort wine.f90 selectn.f90 spoiled.f90 -o wine.x
run:
	./wine.x
edit:
	vim wine.f90
```

codes/wine/Makefile

- To compile codes using make utility: make ↵
  ("make" utility will read the default file "Makefile".)
- Equivalent to: make␣all ↵
- To execute "wine.x": make␣run ↵
- "all" and "run" are called **targets**.
- The line below each target should start with **Tab**, followed by **command**.
- Target name "all" can be changed to one corresponding a project such as "WineProject" (case-sensitive).

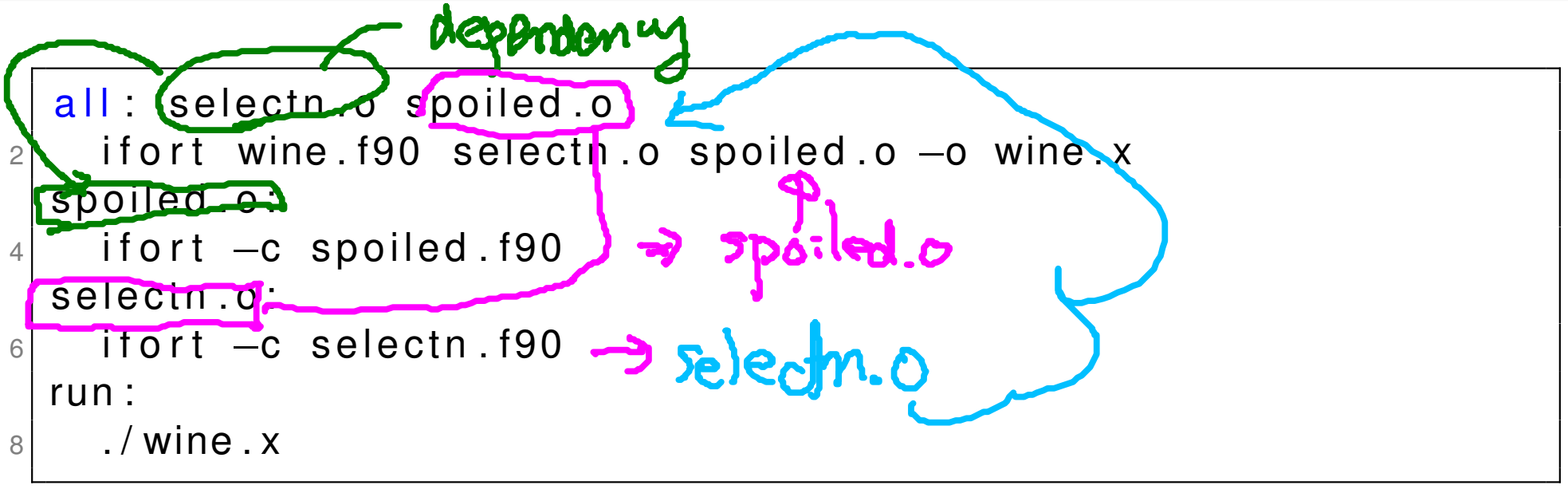
Makefile.1

```
all:
	ifort wine.f90 selectn.f90 spoiled.f90 -o wine.x
run:
	./wine.x
```

codes/wine/Makefile.1

- The same content is stored in “Makefile.1”
- Equivalent to: $ make **-f Makefile.1** all ↵
- To execute “wine.x”: $ make **-f Makefile.1** run ↵

Makefile.2



codes/wine/Makefile.2

- Again
  “$␣make␣-f␣Makefile.2 ↵” and
  “$␣make␣-f␣Makefile.2␣all ↵” are identical.
- Dependency for target: when a target is made, dependencies will be made **first** (if not made).

Makefile.3

```
1  all: lib
       ifort wine.f90  -L./ -lwine -o wine.x
3  # ifort wine.f90  libwine.a -o wine.x
   lib: selectn.o spoiled.o
5    ar -r -v libwine.a selectn.o spoiled.o
   spoiled.o:
7    ifort -c spoiled.f90
   selectn.o:
9    ifort -c selectn.f90
   run:
11   ./wine.x
   clean:
13   rm -f selectn.o spoiled.o libwine.a wine.x
```

codes/wine/Makefile.3

- “libwine.a” library is made using dependencies.
- “clean” **removes** all generated files, except source and Makefile(s).