



UNIVERSIDAD NACIONAL DEL CALLAO
FACULTAD DE CIENCIAS NATURALES Y MATEMÁTICA
FÍSICA COMPUTACIONAL 2

Tarea 1

Tu nombre

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Problema 1

- Enunciado del problema.
- Datos:
 - Lista de cantidades dadas o información proporcionada.
 - Puedes incluir tablas de datos si es necesario.
- A encontrar:
 - Lista de cantidades o resultados a encontrar.

Solución:

Ecuaciones aquí

(1)

```
1 ! Codigo Fortran aqui
2 PROGRAM ejemplo
3   IMPLICIT NONE
4   INTEGER :: i, n
5   REAL :: x, sum
6
7   n = 100
8   sum = 0.0
9
10  DO i = 1, n
11    x = REAL(i)
12    sum = sum + x**2
13  END DO
14
15  PRINT *, 'La suma de los cuadrados es: ', sum
16
17 END PROGRAM ejemplo
```

Preguntas de Programación

1. ¿Qué modificaciones harías al código anterior para calcular la suma de los cubos en lugar de los cuadrados?
2. ¿Cómo podrías generalizar el código para calcular la suma de las potencias n-ésimas de los números enteros del 1 al m?

$$x_{n+1} = x_n - m f(x) \left[\frac{x_n - x_{n-1}}{f(x_n) - f(x_{n-1})} \right] \quad (2)$$

For $m = \frac{1+\sqrt{5}}{2} = 1.618$

Steps	xa	xb	xi	f(xi)	(xn+1-xn)
0	1.500000000000	1.600000000000	1.633191538329	-0.001945949763	0.033191538329
1	1.600000000000	1.633191538329	1.564416498720	-0.000020351034	0.068775039609
2	1.633191538329	1.564416498720	1.563240412447	-0.000028545785	0.001176086273
3	1.564416498720	1.563240412447	1.569869184045	-0.000000429797	0.006628771598
4	1.563240412447	1.569869184045	1.570033141259	-0.000000291226	0.000163957214
5	1.569869184045	1.570033141259	1.570590682342	-0.000000021145	0.000557541083
6	1.570033141259	1.570590682342	1.570661309883	-0.000000009115	0.000070627541
7	1.570590682342	1.570661309883	1.570747894571	-0.000000001173	0.000086584688
8	1.570661309883	1.570747894571	1.570768583633	-0.000000000385	0.000020689062
9	1.570747894571	1.570768583633	1.570784932394	-0.000000000065	0.000016348761
10	1.570768583633	1.570784932394	1.570790299953	-0.000000000018	0.000005367559
11	1.570784932394	1.570790299953	1.570793673498	-0.000000000004	0.000003373545
12	1.570790299953	1.570793673498	1.570794985787	-0.000000000001	0.000001312289
13	1.570793673498	1.570794985787	1.570795714281	-0.000000000000	0.000000728494

A point in the Y-axis represents the measured performance GFLOP/s. This performance number can be compared against the bounds set by the peak compute performance (Peak GFLOPs) and the memory bandwidth of the system (Peak GB/s) to determine what is limiting performance: memory or compute[1].[2]

SCIENTIFIC PROGRAMMING LANGUAGE

Appendices

A Front-end and Back-end

In software engineering, the terms **front-end** and **back-end** refer to the separation of concerns between the presentation layer (**front-end**), and the data access layer (**back-end**) of a piece of software, or the physical infrastructure or hardware. Therefore in a HPC,

- The login servers are called **front-ends** because you do not run your calculations there.
- Rather run your calculations on **back-end** compute servers.
- The **front-end** server provides access to compute servers via the **batch** system, using the **qsub** command.

B Hard Link or Symbolic Link

The **ln** command is a Linux/Unix command used to create file links to an existing file.

B.1 Link types

- There are two types of links
 1. **hard links:** Refer to the specific location of physical data. A hard link allows multiple filenames to be associated with the same file since a hard link points to the inode of a given file, the data of which is stored on disk.
 2. **symbolic links:** Refer to a symbolic path indicating the abstract location of another file. A symbolic links are special files that refer to other files by name.
- The **ln** command by default creates hard links, and when called with the command line parameter **ln -s** creates symbolic links.
- Most operating systems prevent hard links to directories from being created since such a capability could disrupt the structure of a file system and interfere with the operation of other utilities.
- The **ln** command can however be used to create symbolic links to non-existent files.

B.2 Examples

1. Example 1

```
$ ln -s source_file target_file
```

```
$ ls -l source_file target_file
```

```
-rw-r--r-- 1 veryv wheel 0 Mar 7 22:01 source_file
lrwxr-xr-x 1 veryv wheel 5 Mar 7 22:01 target_file -> source_file
```

2. Example 2 - Create a symbolic link for /home/Desktop/Links/Example/example.cpp as /home/Test/example.cpp, copy paste the following command

```
$ ln -s /home/Desktop/Links/Example/example.cpp /home/Test/example.cpp
```

```
$ ll
lrwxrwxrwx 1 vivek vivek      16 2007-09-25 22:53 example.cpp -> /home/Desktop/Links/
Example/example.cpp
```

C Securely Copy (SCP) Files

SCP allows files to be copied to, from, or between different hosts (between a local host and a remote host or between two remote hosts.). It uses `ssh` for data transfer and provides the same authentication and same level of security as `ssh`.

1. Copy the file `foobar.txt` from a remote host to the local host

```
$ scp your_username@remotehost.edu:foobar.txt /some/local/directory
```

2. How to `scp` a file to LANL-IC turquoise/

```
$ scp filename username@wtrw.lanl.gov:username@gr-fe.lanl.gov:/remote/path/to/file
```

3. Also shorter probably works

```
scp filename wtrw:gr-fe:/remote/path/to/file
```

References

- [1] N. Ding and S. Williams. An instruction roofline model for gpus. In *2019 IEEE/ACM Performance Modeling, Benchmarking and Simulation of High Performance Computer Systems (PMBS)*, pages 7–18, 2019.
- [2] Charlene Yang, T. Kurth, and S. Williams. Hierarchical roofline analysis for gpus: Accelerating performance optimization for the nersc-9 perlmutter system. *Concurrency and Computation: Practice and Experience*, 32, 2020.