

MPI Labs - Supplementary material

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Loading modules in the cluster

Basic commands on how to use Environment Modules in the cluster:

```
$ module list  
$ module purge  
$ module load  
$ module spider [module_name]  
$ module unload
```

[Click here to open Environment Modules Documentation](#)

Loading modules in the cluster

In this practice we will need to load a specific version of the GNU compiler and the OpenMPI software to access the MPI compiler, libraries and runtime:

```
$ module spider openmpi
```

```
-----  
openmpi: openmpi/5.0.3  
-----
```

Description:

Open MPI is a powerful and widely-used ...

You will need to load all module(s) on ...

gcc/13.3.0

gcc/8.5.0

Loading modules in the cluster

In this practice we will need to load a specific version of the GNU compiler and the OpenMPI software to access the MPI compiler, libraries and runtime:

```
$ module load gcc/13.3.0  
$ module load openmpi/5.0.3  
$ module list
```

Currently Loaded Modules:

1) gcc/13.3.0 2) openmpi/5.0.3

This is needed every new login!

We can do better...

Loading modules in the cluster

A good practice when working with multiple modules, which can vary depending on the job to launch, is to load modules in your batch script (job.sh):

```
#!/bin/bash
```

```
#SBATCH --job-name=test
```

```
#SBATCH --output=job_%j.out
```

```
#SBATCH --error=job_%j.err
```

```
#SBATCH --partition=std
```

```
#SBATCH --ntasks=4
```

```
#SBATCH --time=00:00:05
```

```
module purge
```

```
module load gcc/13.3.0 openmpi/5.0.3
```

```
mpirun -np 4 <exec> [args] # or srun <exec> [args]
```

What is asked to do?

- 1 Start the `montecarlo.c` source file with a MPI “Hello World” implementation.
- 2 Use the “Hello World” to start testing the Makefile and job submission in the `pirineus3` cluster.

Makefile

Makefile from Cholesky:

```
CC=gcc
```

```
CFLAGS=-O2 -fopenmp -march=native -lm -std=c99
```

```
OBJ=cholesky
```

```
all:
```

```
    $(CC) main.c $(OBJ).c -o $(OBJ) $(CFLAGS)
```

```
clean:
```

```
    rm $(OBJ)
```

Reminder of the SBatch directives to ask for more than one process:

Option 1 (simpler for what we will need)

```
#SBATCH --ntasks=number
```

Option 2 (more control over resource allocation)

```
#SBATCH --nodes=number
```

```
#SBATCH --tasks-per-node=number
```


Monte Carlo Exercise

What is asked to do?

- 1 Start the `montecarlo.c` source file with a MPI “Hello World” implementation.
- 2 Use the “Hello World” to start testing the Makefile and job submission in the `pirineus3` cluster.
- 3 Read the 3 command line arguments:
`N`, `NUM_SAMPLES`, `SEED`
- 4 Distribute the number of points to compute among the number of processes.
- 5 Generate random (x_1, x_2, \dots, x_i) coordinates over the hypercubed domain. HINT: Number generator $x \in [0, 1]$, then in order to get $x \in [-1, 1] \rightarrow x = 2 * x - 1$.

What is asked to do?

- Count the number of points are inside the hypersphere:

$$\sqrt{x_1^2 + x_2^2 + \cdots + x_i^2} \leq 1 \text{ for } i = 1, Dims$$

- After the counting, do you need any MPI communication?
What about the timings?
- Every MPI process has to time the Monte Carlo computation, and only the slowest must be printed. Again, any MPI communication needed?

Flight Controller: Understanding the problem

Before starting to code we need to properly understand the problem and how it's coded:

1. Explore input data

```
# Plane Data
# Map: 100.00, 50.00 : 10 5
# Number of Planes: 5
# i x y vx vy
0 10.0 1.0 0.0 1.0
1 30.0 1.0 0.0 1.0
2 50.0 1.0 0.0 1.0
3 70.0 1.0 0.0 1.0
4 90.0 1.0 0.0 1.0
```

Flight Controller: Understanding the problem

Before starting to code we need to properly understand the problem and how it's coded:

1. Explore input data
2. Create Makefile and job.sh for sequential program

```
CC=...  
CFLAGS=-O3 -lm -std=c99  
OBJ=...  
OBJ2=...
```

```
seq:  
    ...
```

```
par:  
    ...
```

```
clean:  
    rm $(OBJ) $(OBJ2)
```

Flight Controller: Understanding the problem

Before starting to code we need to properly understand the problem and how it's coded:

1. Explore input data
2. Create Makefile and job.sh for sequential program
3. Learn how to run it

```
./fc_seq input_planes_test.txt ...  
Flight controller simulation: ...  
Time: comp: 0.00s      total: 0.00s  
Ok! Plane 0 found at (10.00, ...)  
Ok! Plane 1 found at (30.00, ...)  
Ok! Plane 2 found at (50.00, ...)  
Ok! Plane 3 found at (70.00, ...)  
Ok! Plane 4 found at (90.00, ...)
```

Flight Controller: Understanding the problem

Before starting to code we need to properly understand the problem and how it's coded:

1. Explore input data
2. Create Makefile and job.sh for sequential program
3. Learn how to run it
4. Navigate the code

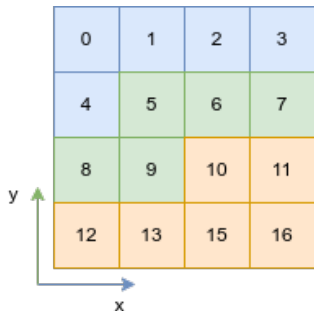
```
./fc_seq input_planes_test.txt ...  
Flight controller simulation: ...  
Time: comp: 0.00s      total: 0.00s  
Ok! Plane 0 found at (10.00, ...)  
Ok! Plane 1 found at (30.00, ...)  
Ok! Plane 2 found at (50.00, ...)  
Ok! Plane 3 found at (70.00, ...)  
Ok! Plane 4 found at (90.00, ...)
```

Flight Controller: Understanding the problem

Before starting to code we need to properly understand the problem and how it's coded:

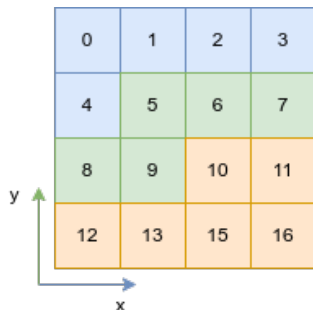
- | | |
|--|---|
| 1. Explore input data | |
| 2. Create Makefile and job.sh for sequential program | <pre>./fc_seq input_planes_test.txt ...
Flight controller simulation: ...
Time: comp: 0.00s total: 0.00s
Ok! Plane 0 found at (10.00, ...)
Ok! Plane 1 found at (30.00, ...)
Ok! Plane 2 found at (50.00, ...)
Ok! Plane 3 found at (70.00, ...)
Ok! Plane 4 found at (90.00, ...)</pre> |
| 3. Learn how to run it | |
| 4. Navigate the code | |
| 5. Navigate the MPI code, check TODOs | |

Flight Controller: Domain decomposition



- Map Grid $N \times M$: 4×4
- MPI Comm Size = 3
- How do we decompose the domain?
- `total_displacements[size+1]`
- Each process start at index:
 $i * (\text{gridCells}) / \text{size}$
- And takes the following number of cells:
`total_displacements[i+1] - total_displacements[i]`

Flight Controller: Domain decomposition

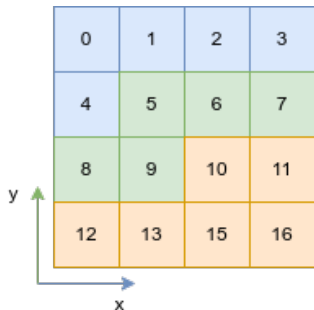


$$i * (\text{gridCells}) / \text{size}$$

- $i = 0 * 16 / 3 = 0$
- $i = 1 * 16 / 3 = 5$
- $i = 2 * 16 / 3 = 10$
- $i = 3 * 16 / 3 = 16$

i=0	i=1	i=2	i=3
0	5	10	16

Flight Controller: Domain decomposition



How many grid cells are required for a process?

- Rank 0 $\rightarrow 5 - 0 = 5$ Starts 0
- Rank 1 $\rightarrow 10 - 5 = 5$ Starts 5
- Rank 2 $\rightarrow 16 - 10 = 6$ Starts 10

i=0	i=1	i=2	i=3
0	5	10	16

Flight Controller: Reading planes with MPI

What is expected in the function `read_planes_mpi`?

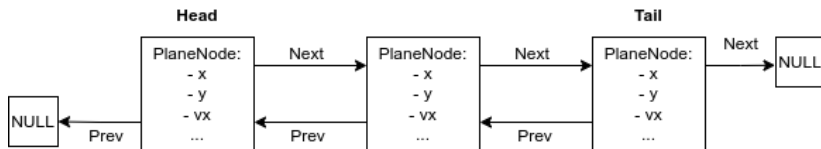
- 1 Review and understand the sequential reading.
- 2 Use the sequential version as a base code.
- 3 Distribute the grid cells among the processors using the variable: `tile_displacements`
- 4 For each rank, only the planes that are in its domain should be inserted to `PlaneList`.

Flight Controller: Reminder double-linked list

Planes are stored by every process in a **double-linked list**.
Although, its canonical functions are implemented, such as:

- `insert_plane`
- `remove_plane`
- `seek_plane`

It's key to remember how to work with the list:



What is expected in the function `communicate_planes_send`?

- ① Count how many planes I have to send, and to who? HINT: `get_rank_from_index`
- ② Communicate with the group what I need to send and what I have to receive.
- ③ Send planes that are out of my domain and remove them from my current list. HINT: allocate buffers for an async send.
- ④ Receive planes from the rest of the group and add them to my list.

Flight Controller: Async Send buffers

In a Non-blocking MPI Send, the application sending buffers should remain untouched until the communication finishes. . . Then, we have to allocate memory for every rank we are sending planes to:

