Preparing your environment for the practical

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1 Login to the cluster

• It may be useful to open the documentation of Smilei in the web browser:

http://www.maisondelasimulation.fr/smilei

In particular, the documentation explaining the entries of the input namelist (but normally you should find all the necessary explanations in the handouts):

https://smileipic.github.io/Smilei/namelist.html

- Open a shell/Terminal window to work on command line
- Login to the Ruche cluster and then enter your password, which will not appear on your screen (see the access credentials you have received):

```
ssh -XY username@...
```

Once you are connected you will be in your home space, whose path is also referenced with the shortcut \$HOME. It is highly recommended to use this space only to compile the code. As explained in the following, run your simulations in the space called \$WORKDIR.

2 Compile the code Smilei

• Download Smilei:

git clone https://github.com/SmileiPIC/Smilei.git
and then enter the newly created folder Smilei:
cd Smilei

- Clean potentially incomplete build files: make clean
- Compile the code from the code folder:

make -j 10 machine=ruche

This should create the files called smilei and smilei_test. If you see the line Linking

smilei_test for test mode and no errors are displayed, everything should have worked well. It is normal to see messages like In file included from ...

- Compile the postprocessing library happi: make happi
- To know the location of your executable file, just use: pwd

This command will display the path to your current working directory, for example path/to/executable. This path will be used later. Now your executables smilei and smilei_test should be found in your folder path/to/executable.

3 Prepare your simulation

- Enter your working space:
 cd \$WORKDIR
- Create a new directory sim where you will run your simulation: mkdir sim cd sim
- Inside this folder, create a link to the executables:

ln -s path/to/executable/smilei

ln -s path/to/executable/smilei_test

The expression path/to/executable is just an example, you will need to insert the path where your files smilei and smilei_test are.

- Inside this folder, you will need a file to submit a simulation job to the job scheduler, e.g. submission_script.sh. You can transfer the file you already have through scp or just copy and paste it in a new file inside your simulation folder.
- Inside this folder, you will need also the input file of your simulation InputNamelist.py. Once you have all these files in your simulation folder (executables, submission script, input namelist) you are ready to run your simulation. If you change the name of your namelist, remember that it must be a .py file and it must appear a the end of the submission_script.sh.

4 Run your simulation

• IMPORTANT WARNING: do NOT launch a simulation directly, always use a simulation job submission script as described below. You are now connected in the login nodes of the cluster, made to transfer files and compile codes, and shared among the connected users. If you launch a simulation directly it will be run on this shared space where all the machine users can connect, slowing down or blocking their operations. Imagine to have a very slow home wifi connection, sufficient only to send some e-mails to work, shared among you and many house-mates. In this analogy running a simulation directly on the login node is equivalent to start a long video-call, blocking everyone elses' attempt to send e-mails and work properly.

Instead, launching a simulation with a job submission script as described in the following will make the simulation run on the compute nodes, where the necessary resources are safely distributed among the machine users. Science is also learning to work together and to respect each other's space.

• Check if you have all the required files (executables, submission script, input namelist) through the command:

ls

• To check that your namelist does not contain syntax errors, use the **smilei_test** executable on the namelist (you'll need to load the same libraries used for the code compilation):

```
./smilei_test InputNamelist.py
```

If you see the line END TEST MODE, the namelist does not contain syntax errors and can be run.

• Launch your simulation job:

```
sbatch submission script.sh
```

• To check the status (running/queueing etc) of yout job:

```
squeue -u $USER
```

This should also give you the number JobId of your job, necessary for the next command.

• To delete your job from the queue:

```
scancel JobId
```

• To read the end of the log file and let it refresh (if you want to watch your simulation execute for example):

```
tail -f smilei.log
```

ctrl+C will allow you to stop watching the file refresh.

• If you want to change the time you want for your simulation, change the corresponding line in the file submission_script.sh (here 20 minutes):

```
#SBATCH -time=00:20:00
```

The longest simulation of the session runs approximately for 3 minutes with 10 MPI processes and 2 OpenMP threads. These parameters are already set in the submission script.

• If you want to change the number of OpenMP threads in your simulation, change the corresponding line in the file **submission_script.sh** (here 2 threads):

```
export OMP_NUM_THREADS=2
```

• If you want to change the number of MPI process in your simulation, change the corresponding line in the file **submission_script.sh** (here 10 processes):

```
#SBATCH -ntasks=10
```

5 Postprocess your simulation results

- Open IPython (before, you will need to load the Python modules and define variables like how you did to compile the code, and be sure you have compiled happi): ipython
- Import the libraries you need:

```
import happi
import numpy as np
import matplotlib.pyplot as plt
```

The output files have the extension .h5 and can be opened with the postprocessing library happi. You will need also the file smilei.py, generated at the start of your simulation.

• Open your simulation:

```
S = happi.Open("path/to/my/results")
again, "path/to/my/results" is an example, you will need to put the path of your simulation.
```

If you use simply S = happi.Open(), the library happi will open the results inside the current working directory.

• Now you can use the commands in the section **Crash course on the happi postprocessing library** in the handouts.

6 Command line cheatsheet

- pwd : shows the path of the current working directory.
- cd path : go to path
- ls: see the content of the current directory.
- 1s path: see the content in path.
- rm file: removes file. To remove a folder, you will need an additional flag: rm -r folder.
- cp source_file destination_path: copies source_file to the destination_path.
- scp source_file destination_path: same as cp, but you can also transfer folders and files to a different machine, e.g. from the cluster to your computer and vice versa. You will be asked to provide your username, the server address and your password, e.g. scp source_file username@server:/destination_path/. This command can be used to transfer output files from the cluster to your computer for later postprocessing if so you prefer (of course larger data files will need more time to transfer).
- mv source destination: move source (can be a file or directory) to a destination. If the destination does not specify a path, the command renames source with the name destination.
- ipython: opens Ipython, where also the previous commands can be used. To run a Python script inside this interface, use %run script_name.py.