Testing Quantum ESPRESSO, LAMMPS and the Virtual Machine

The labs will rely on your ability to run calculations on a virtual machine on your personal computer. For this reason, we would like you to test to see (a) if the VM is correctly set up and (b) your machine is powerful enough to complete the exercises.

To perform the tests, follow the instructions below:

- Download the test files from: https://drive.google.com/file/d/1BCsC7pS7HymmZZimINF-wnb8jIzL5ktW/view?usp=sharing

- Move the test files inside the VM using the shared folder (that you set up as explained in the instructions).
    - For Macbook users with Apple M chip, you can alternatively copy the files in the virtual machine using scp from your local terminal, using:

      `scp -P 2200 Downloads/test.zip max@127.0.0.1:`

  Alternatively, you can just open a browser inside the VM, and download the file directly inside the VM, so you don't need to transfer them via the shared folder or via scp.
- Inside the Virtual Machine, uncompress the test files by either:
    - right clicking the zipped file and choosing the appropriate option to unzip it “Extract here” (this will put the files in a subfolder)
    - running in the command line: `unzip test.zip`
- Inside you will see 2 folders.
- Open the LAMMPS folder in a terminal by either:
    - Open a terminal and change into the directory where `Ni_md.in` is located (using the command `cd`).
    - From the folder where `Ni_md.in` is located, right click and choose “Open in terminal”.
- Run the following command in the terminal:

  mpirun -np 2 lmp_mpi -in Ni_md.in > Ni_md.out
- This will outputs 5 files -
    - Ni_md.out - contains time, temperature, KE, PE and pressure plus a bunch of other info from LAMMPS
    - positions.lammpstrj - contains the scaled coordinates of all the atoms
    - velocities.lammpstrj - contains the velocities of all the atoms
    - recovery.dat - recovery file that can be used to start the calculation from last positions and velocities
    - log.lammps - log file
- Open the `Ni_md.out` file and look towards the end for the line like this (use the one mentioning 30000 steps, there is a similar line in the beginning mentioning 5000 steps):

  `Loop time of 2.83772 on 2 procs for 30000 steps with 500 atoms`

  The number after “loop time” is the time the calculation took (in this example above written in red, 2.83772 seconds) that you need to report in the LAMMPS section of the form linked later in this document.
- Open the folder QE in a terminal by either:
    - Open a terminal and change into the directory where `test.in` is located (using the command `cd`).
    - From the folder where `test.in` is located, right click and choose “Open in terminal”.
- **IMPORTANT FOR THE NEXT STEP: Do not run Quantum ESPRESSO directly inside the shared folder.** This will create problems because some files get wrong permissions and cannot be deleted anymore (and your calculations will crash!) **Run anywhere else (e.g. on the Desktop of your VM).** Then, at the end, you can copy relevant inputs and outputs to the shared folder, if you need to copy them out.
- Run the command:

  `pw.x < test.in > test.out`
- Wait for the command to finish. It should take a couple of minutes at most.
- Open the `test.out` file with any text editor, and look at the end for a line that should look like this:

```
PWSCF        :      59.67s CPU   1m 0.53s WALL
```

The number before “WALL” is the time the calculation took (in this example above written in red, 1 minute and 0.53 seconds) that you need to report in the QE section of the form linked below.

Regardless of whether or not you were able to complete the above steps successfully, please complete the following google form:
https://docs.google.com/forms/d/e/1FAIpQLSdIL6o4IKARztQtI09heOZ8Hpv8i-ULvOUnO94B3BIdoTY4Ew/viewform?usp=dialog
Before Thursday 27th February evening *(you will need to be logged into Google with your EPFL account to access this form).*

If there is a problem, we will get in touch with you in order to resolve any issues before the lab sessions begin.

Good luck!