TEL AVIV UNIVERSITY   SCHOOL OF PHYSICS AND ASTRONOMY

Exercises for

Computational Modeling of Quantum Materials

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Pre-exercise preparations

1. Basics in shell scripting

The density functional theory (DFT) package that we will be using (VASP) runs on Linux and we will therefore be using the unix shell. Please familiarize yourself with basic shell commands, as well as basic shell tools (grep, sed, awk) for input/output formatting. A list of tutorials can be found below, but you may use any you can find on the web.

- Basic shell script tutorial including the grep command (extracing data from files):
  https://swcarpentry.github.io/shell-novice/

- More basic shell including ssh (for remote access) and awk (for processing text):
  https://carpentries-incubator.github.io/shell-extras/

- Basic shell script tutorial:
  https://www.learnshell.org/

- Sed tutorial (file manipulation):
  https://www.geeksforgeeks.org/sed-command-in-linux-unix-with-examples/

- Detailed awk tutorial, for the motivated:
  https://www.tutorialspoint.com/awk/index.htm

- Detailed shell script tutorial, for the motivated:
  https://www.shellscript.sh/index.html

If you have no prior knowledge of using the shell, I would advise to at least work through the first tutorial in the above list before the first exercise.

2. Postprocessing and plotting

Some of the data we produce with the DFT calculations will need to be postprocessed and plotted with programs beyond the basic shell tools. You may use a program or programming language of your choice to do so (Python, Mathematica, Matlab, ...).

3. Remote access to the workstation

You will use your laptops to access the workstation in order to run density functional theory calculations with VASP. To enable access, you will need a TAU VPN connection.

- Step-by-step introduction for TAU VPN:
  https://computing.tau.ac.il/helpdesk/remote-access/communication/vpn
  This involves setting up Google Authenticator on your phone for two-step authentification and installing GlobalProtect VPN on your laptop.

Once you're connected to the university's network through VPN, open the terminal and connect to the workstation:

```
$ ssh USERNAME@132.66.128.97
```

Your username is the same as your TAU login name (usually what's leading your email address USERNAME@mail.tau.ac.il). The password is your student ID. You will be asked to set a new password right away, please remember the password you are setting here! Once logged in, run a test with VASP to see whether everything works. In order to do so, create and go to the Calculations directory in your home directory

```
$ mkdir Calculations
$ cd Calculations
```

and copy the test folder to that directory,

```
$ cp -r /home/vasp_input/test_BFO .
```

Enter the directory

```
$ cd test_BFO
```

and run the executable for vasp by typing the following command:

```
$ mpirun -n 2 /home/dominik/Dominik/VASP/vasp.6.3.2/bin/vasp_std
```

You will see some output produced in the terminal and as files in your current directory. If the last line of the terminal output begins with "1 F=", followed by some numbers, everything works as it should. You can now delete the test files and folder, as we will be using different examples in the exercise:

```
$ cd ..
$ rm -rf test_BFO
```

Complete this test before the beginning of next lecture so that we are all on the same page. If something doesn't work, please contact me per email and describe the problem. (It may be that some permissions are set incorrectly, which we would need to fix before the exercise.)