Post-processing and analysis

Gabriel Antonius

Université du Québec à Trois-Rivières, Canada

Abinit School 2026

What is Abipy

- Scripts that can be executed on the command line for a quick vizualisation of Abinit results.
- Objects and functions to extract data from Abinit output files and plot it.
- Objects and functions to create workflows and execute them.

Setup

We will be working with the Abipy package, which requires some setup.

Copy the abipy configurations files in your home directory:

```
cp -r $ABISCHOOL/.abinit ~/
```

Copy the abipy examples:

```
cd $CCCWORKDIR
cp -r $ABISCHOOL/abipy_examples .
```

The Abipy documentation

We will rely on three sources of documentation:

1. The examples in the `abipy_examples` directory that you have copied (also found in the source code: https://github.com/abinit/abipy).
2. The Abipy notebook tutorials found here: https://abinit.github.io/abipy_book
3. The Abipy API documentation found here: https://abinit.github.io/abipy

For this training session

We want you to consult the abipy notebook tutorials and write your own scripts to accomplish the **objectives** listed hereafter.

The following sections of the Abipy notebook tutorials will help you:

- **Output Files**
  - The GSR file (Ground-State Results)
  - The HIST.nc file (relaxation/MD)
- **AbiPy Workflows**
  - Tasks, Workflows and Flow
- **AbiPy Lessons**
  - Base1 lesson (H2 molecule)
  - Base3 lesson (silicon)

Do not read them from start to finish! Try to extract the information that you need to complete the objectives.

Objectives (I)

Write small python scripts to:

- Plot a convergence study with respect to `ecut`.
- Plot a convergence study with respect to `nkpt`.
- Plot a band structure and a density of states (DOS).
- Plot the evolution of the maximum force and total energy in a relaxation.

Make sure that you are able to customize those scripts, e.g. by setting the title, the line colors, etc.

Objectives (II)

Write and execute a workflow to:

- Compute the electronic band structure of silicon.
- Compute the energy of the H_2 molecule as a function of distance.
- Perform a relaxation of aluminium.
- Perform a convergence study of aluminium with respect to k-points and `tsmear`.
  - Then write a script to plot the k-points convergence for the different values of `tsmear` on the same graph.

The solutions to these tests are placed in this directory:
`$ABISCHOOL/abipy_tutorial_solutions/`