

How to get the Abinit executables

The Abinit executables are located in `/home/nfs3/smr3191/Abinit/bin`

To prepare the execution of the tutorials, please follow the following two steps:

Copy the directory with the executables inside your `/scratch/$USER` with:

```
cd /scratch/$USER
cp -r /home/nfs3/smr3191/Abinit/local/bin abinit_bins
```

Add this directory to your `$PATH` with:

```
export PATH=/scratch/$USER/abinit_bins:$PATH
```

Now it's possible to invoke the executables without having to type the absolute path. Try e.g.

```
abinit -v
```

to get the Abinit version (8.7.7) and:

```
abinit -b
```

to list the options activated during the build.

How to get the input files for the lessons

The input files for the tutorials are in `/home/nfs3/smr3191/Abinit/github_abinit/tests/`. For efficiency reasons, we suggest to run the tutorials inside the scratch directory. To do so, create an `abinit/tests` directory inside `/scratch/$USER` with the following commands:

```
cd /scratch/$USER
mkdir abinit
cd abinit
mkdir tests
cd tests
```

Finally, copy the input files for the tutorials with:

```
cp -r /home/nfs3/smr3191/Abinit/github_abinit/tests/ .
```

Then cd to the directory containing the input files for the DFPT lessons:

```
cd tests/tutorespfn/
```

Now you can start to follow the RF1 lesson on the Abinit web page <https://docs.abinit.org/tutorial/rf1>

Remember to replace all the occurrences of `~abinit/` in the examples with `/scratch/$USER/`

The code has been compiled with MPI and netcdf support. For the configuration options, see the `ictl_conf.ac` autoconf file (usage: `./configure --with-config-file=ictl_conf.ac``).

To run the code in parallel, e.g. with 4 MPI processes, use:

```
mpirun -n 4 abinit < files_file > run.log 2> run.err &
```

How to run the tdepes tutorial

The tutorial on temperature dependent band structures is available at <https://docs.abinit.org/tutorial/tdepes/>. The examples require a python script to read the netcdf files produced by Abinit and analyze the data. The python code can be found in `/home/nfs3/smr3191/Abinit/scripts`.

If you are running on the ICTP machines, you need to activate a [conda](#) environment that will provide all the required dependencies. Use:

```
source /home/nfs3/smr3191/Abinit/miniconda3/bin/activate env2.7
```

to work in the `env2.7` conda environment (the prompt will change, use `which python` ...) Then follow the instructions available on the Abinit website.

Note that there's a typo in the documentation as the `plot_bs.py` script is inside the `post_processing` directory and not in `temperature-dependence`. Use:

```
cp /home/nfs3/smr3191/Abinit/scripts/post_processing/plot_bs.py .
```

to copy the script.

Important

The `plot_bs.py` script uses [matplotlib](#) to plot the band structure with the electron-phonon renormalization. The script will try to use the X-server to display the figure.

Remember to use the `-Y` option to connect to the machine e.g.

```
ssh user@ssh.ictp.it -Y
user@ssh-2 ~ $ ssh hp83-inf-22 -Y
```

This option is needed to avoid the X-server error:

```
File "/home/nfs3/smr3191/Abinit/miniconda3/envs/env2.7/lib/python2.7/site-
packages/matplotlib/backends/backend_qt5.py", line 125, in _create_qApp
    raise RuntimeError('Invalid DISPLAY variable')
```

AbiPy-based lesson

To use the [AbiPy](#) tools on the ICTP machines, you need to activate the `env3.6` conda environment with:

```
source /home/nfs3/smr3191/Abinit/miniconda3/bin/activate env3.6
```

Now create a new directory and copy the two yaml files required to launch calculations:

```
mkdir abipy_test && cd abipy_test
cp /home/nfs3/smr3191/Abinit/abipy_examples/scheduler.yml .
cp /home/nfs3/smr3191/Abinit/abipy_examples/manager.yml .
```

Validate the installation with:

```
abichk.py --with-flow
```

To launch your first AbiPy flow, use the `run_si_ebands.py` script:

```
cp /home/nfs3/smr3191/Abinit/abipy_examples/run_si_ebands.py .  
  
# Build flow directory  
./run_si_ebands.py  
  
# Run the flow with abirun  
abirun.py flow_si_ebands/ scheduler
```

The HTML version is available [here](#). Additional examples can be found in the [Flow gallery](#). Use:

```
abirun.py --help
```

to get the list of commands.

Now you can look at the other lessons available in the [abitutorials package](#)