

Theorist HT Induction Course

Lesson 1: Setting up your new computer (Mac OS X \geq 10.6)

As of 9/27/2012

Caveats

- These are recommended setup steps for Mac OS X \geq 10.6. They are not the only possible setup.
- You may of course choose to ignore any of the steps. But you are on your own in terms of searching the web for advice if any component is not working.
- Since a majority of the theorists uses Macs, these steps are customized for Macs. If you are setting up on Ubuntu machines, many of the steps are trivial with apt-get. If you are setting up on Windows, you probably can get a lot of the packages pre-built.

Step 1: Preparing your Mac

- You will first need to download and install basic compilers:
 1. Xcode – This provides the gcc compiler. Get it from the App Store. After that, go to Preferences->Downloads and install the Command Line Tools. Note that this download and install takes a long while. You may need to quit Xcode and reopen if that does not appear.
 2. Gfortran 4.6.2+. Get an installer at <http://gcc.gnu.org/wiki/GFortranBinaries#MacOS>.

Step 2: Install Python 2.7+

- It is recommended that you install the latest copy of Python 2.7+ (not 3+), even though your Mac should already have a compatible version. This makes it easier for future upgrades and minimizes issues between your Mac's python and what is used for HT work.
- Get it from www.python.org and install.
- Ensure that your terminal is running the correct version by typing "**which python**". You should get something like `/Library/Frameworks/Python.framework/Versions/2.7/bin/python`". If you don't get this (e.g., if you get `/usr/bin/python`), you may need to change your PATH.

Step 3: Install the Python setuptools

- Python setuptools make it easier to install subsequent programs via “easy_install”. If you want to, you can install pip as well using “sudo easy_install pip”. Pip has several advantages over easy_install.
- In terminal, run

```
curl -o setuptools-0.6c11-py2.7.egg  
http://pypi.python.org/packages/2.7/s/  
setuptools/setuptools-0.6c11-py2.7.egg
```

```
sudo sh setuptools-0.6c11-py2.7.egg
```

Step 4: Numpy and Scipy packages

- Download the **tar.gz source code (not the pre-built packages)** for numpy and scipy from <http://www.scipy.org/>. We are compiling from source. For scipy, download 0.10.1. Newer versions seem to have an issue compiling.
- In the terminal, do the following (if your versions are newer, change the version numbers accordingly):

```
tar -zxvf numpy-1.6.2.tar.gz
cd numpy-1.6.2
sudo python setup.py install
tar -zxvf scipy-0.10.1.tar.gz
cd scipy-0.10.1
export CC=gcc-4.2
export CXX=g++-4.2
export FFLAGS=-ff2c
sudo python setup.py install
```

Step 5: Install git and github accounts

- Get a free github account.
 - Add your ssh key (in `$HOME/.ssh/id_rsa.pub`. If it does not exist, create one using “ssh-keygen”) in your account settings.
 - Get Will/Shyue to add you to the Ceder group team.
- Install git from <http://git-scm.com/>.
 - Follow the instructions on this page
 - <https://help.github.com/articles/set-up-git>

Step 6: Clone and setup the relevant Github repos

- **Pymatgen**

```
git clone git@github.com:materialsproject/pymatgen.git
```

From pymatgen directory

```
sudo python setup.py develop
```

- **Pymatpro**

```
git clone git@github.com:materialsproject/pymatpro.git
```

- **Pyabinitio**

```
git clone git@github.com:materialsproject/pymatgen.git
```


Step 7: Install the necessary python dependencies and paths

- PycifRW (for reading cifs)
 - You will need to do this manually since the PyPi version seems to be broken. In the pymatgen directory, go to dependencies/PyCifRW-3.3, type “sudo python setup.py install”.
- pymongo (for db access)
 - Type “sudo easy_install pymongo” or “sudo pip install pymongo”.
- Qhull
 - Download from qhull.org. Follow the instructions in pymatgen’s documentation to install it.
- Add a VASP_PSP_DIR to your environment, e.g., by adding a “export VASP_PSP_DIR=/path/to/potcars” in your .bash_profile. A set of vasp POTCARs have been provided in pyabinitio under the “resources/VASP_PSP” directory.

Step 8: Setup your IDE if desired.

- Eclipse (recommended)
 - <http://www.eclipse.org/downloads/>
 - Download eclipse classic and install.
- Pydev (recommended)
 - <http://sourceforge.net/projects/pydev/files/>
 - Download pydev (not mylyn integration) and install.
- Create new projects with your cloned pymatgen, pymatpro and pyabinitio repos.

Step 9: Familiarize yourselves with git, python and pymatgen

- Learn how to commit and push changes with git. The model is that you should be creating branches for anything that you do, and you should *commit often*.
- Pymatgen has extensive documentation at <http://packages.python.org/pymatgen/>. Read and learn to use it. A hour spent figuring out how to work with pymatgen will save you 100 hours over a year (and probably more as you become more familiar).