Installing Python and packages for Computational Materials Science on MAC

G-Doc available here

Installing MacPorts

1. Follow Directions Here!

Installing Packages

1. Terminal: `sudo port -v selfupdate`
    a. Should not take long if you just installed MacPorts
    b. -v = verbose = tell me what you are doing
2. Install desired packages (Generally in Terminal: sudo port install *pakage_name*)
    a. For General Scientific and Computational work I do as follows:

`sudo port install git`	(track changes - see try.github.com)
`sudo port install python27`	*
`sudo port install py27-pep8`	(Python Com standards checker)
`sudo port install py27-pygtk`	(Graphical interface support)*
`sudo port install py27-pyqt4`	(Graphical interface support)
`sudo port install py27-matplotlib +gtk2`	(plotting tools with gtk support (for ase))
`sudo port install py27-numpy`	(Math)*
`sudo port install py27-scipy`	(Math)*
`sudo port install py27-ipython +notebook`	(I don't use but some people like it see here)
`sudo port install  sudo port install pip`	
`sudo port install vim +python27 +gtk2 +huge`	(text editor - with all the variants)
`sudo port install macvim`	(gui text editor)

(pip is an Installer that may be useful - always check to see if a package is available in MacPorts before installing with pip - just google "Macports package_name")
* - critical for ASE - **pygtk must be installed before matplotlib**

Checking Packages

1. Some packages such as python are preinstalled on your system or have multiple verisions so we need to check that the correct ones are being used.
    a. Terminal:

`sudo port select --list python`	(this list all python packages available)
`sudo port select --set python python27`	(set MacPorts python27 to be active)

sudo port select --set ipython ipython27	(set MacPorts ipython27 to be active)
sudo port select -- list pip	(this list all pip packages available)
sudo port select --set pip pip27	(set MacPorts pip27 to be active)
sudo port select --list vim	(this list all python packages available)
sudo port select --set vim python27	(set MacPorts python27 to be active)

Installing Atomic Simulation Environment (ASE)

1. I am still not 100% this is right
2. Download ASE and put in you home directory
3. Extract it - Terminal: tar -xf python-ase-3.9.0.4465.tar.gz
4. cd into the ase directory - e.g. Terminal: cd $HOME/python-ase-3.9.0.4465/ase
5. Install with python - Terminal: python setup.py install --user
    a. **(I did not use the user option see note below)**
6. Copy all of the files in /tools to your bin file:
   Terminal: sudo cp $HOME/python-ase-3.9.0.4465/ase/tools/* ~/bin/
   (I have not run this… may not be right)
7. Test ase - Terminal:
    a. cd $HOME
    b. bash (using the *bash* shell is suggested on the ASE site - I don't know why)
    c. mkdir /tmp/testase.$$; cd /tmp/testase.*
    d. python -c "from ase.test import test; test(verbosity=2, display=True)" 2>&1 | tee testase.log
    e. I currently end with 2 errors and 1 failure that I am not sure how to fix but it seems to work

FYI:

1. Macports python packages are stored here:
   /opt/local/Library/Frameworks/Python.framework/Versions/2.7/lib/python2.7/site-packages/
2. Note on why to use "--users" - **How to install with python** - i.e packages not in MacPorts
    a. Remove your .pydistutils file if you have one - (?? I don't get this and where is it - I can't find)
    b. python setup.py install --user
        i. do not omit --user and do not use sudo
        ii. This will place user installed packages in ~/Library/Python/2.7/lib/python/site-packages where they will automatically be picked up by the Python installation, without messing up the MacPorts file structure. Note that you can also install packages in a similar way using easy_install-2.7 and pip-2.7 by specifying the --user option.
        iii. The reason for installing packages with --user is that if instead you install packages using sudo python setup.py install, the packages will be installed inside the MacPorts tree, but MacPorts won't be aware of it, so this could cause issues in future if the package is

installed via MacPorts. As a rule of thumb, don't ever install anything into /opt/local/ other than via the port command. If you did mistakenly install packages to the MacPorts directory, just go to/opt/local/Library/Frameworks/Python.framework/Versions/2.7/lib/python2.7/site-packages and remove the files relating to the package you installed.

run test get errors:

```
======================================================================
ERROR: calculator/traj.py (ScriptTestCase)
----------------------------------------------------------------------
Traceback (most recent call last):
  File "/Users/austinfox/ase/ase/test/__init__.py", line 51, in testfile
    {'display': self.display})
  File "/Users/austinfox/ase/ase/test/calculator/traj.py", line 35, in <module>
    os.mkdir(name + '-test')
OSError: [Errno 17] File exists: 'emt-test'

======================================================================
ERROR: fio/oi.py (ScriptTestCase)
----------------------------------------------------------------------
Traceback (most recent call last):
  File "/Users/austinfox/ase/ase/test/__init__.py", line 51, in testfile
    {'display': self.display})
  File "/Users/austinfox/ase/ase/test/fio/oi.py", line 73, in <module>
    assert np.all(np.abs(a1.get_positions() -
AttributeError: 'list' object has no attribute 'get_positions'

======================================================================
FAIL: db.py (ScriptTestCase)
----------------------------------------------------------------------
Traceback (most recent call last):
  File "/Users/austinfox/ase/ase/test/__init__.py", line 51, in testfile
    {'display': self.display})
  File "/Users/austinfox/ase/ase/test/db.py", line 18, in <module>
    assert len(list(con.select())) == 5
AssertionError

----------------------------------------------------------------------
```

refs:

https://astrofrog.github.io/macports-python/
http://klab.smpp.northwestern.edu/wiki/images/e/e6/Macport.pdf