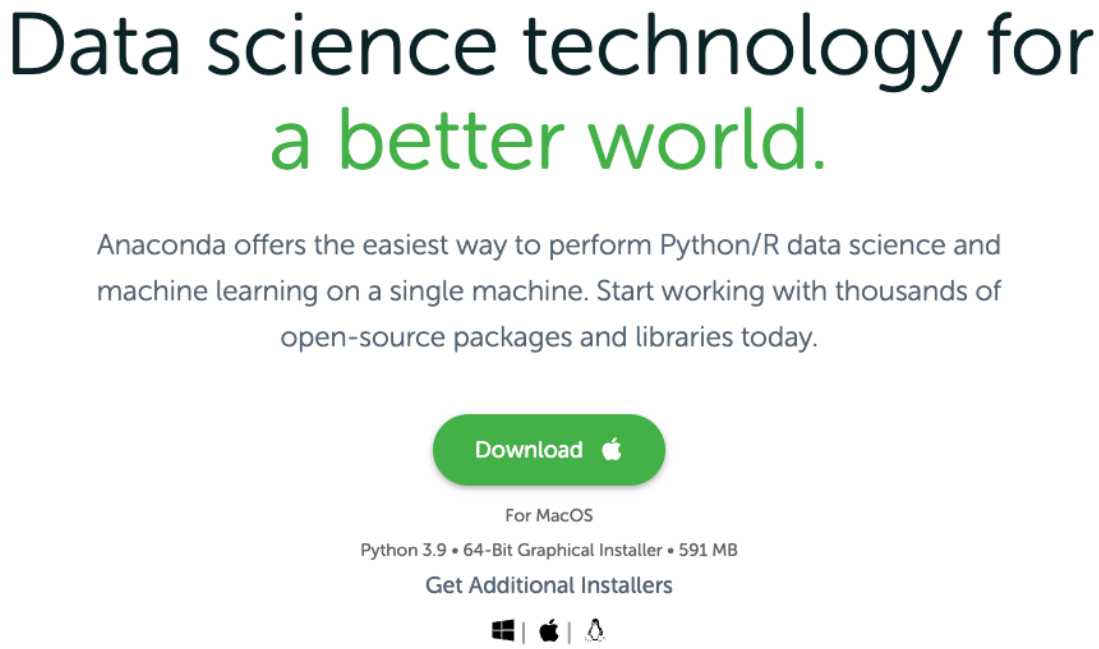
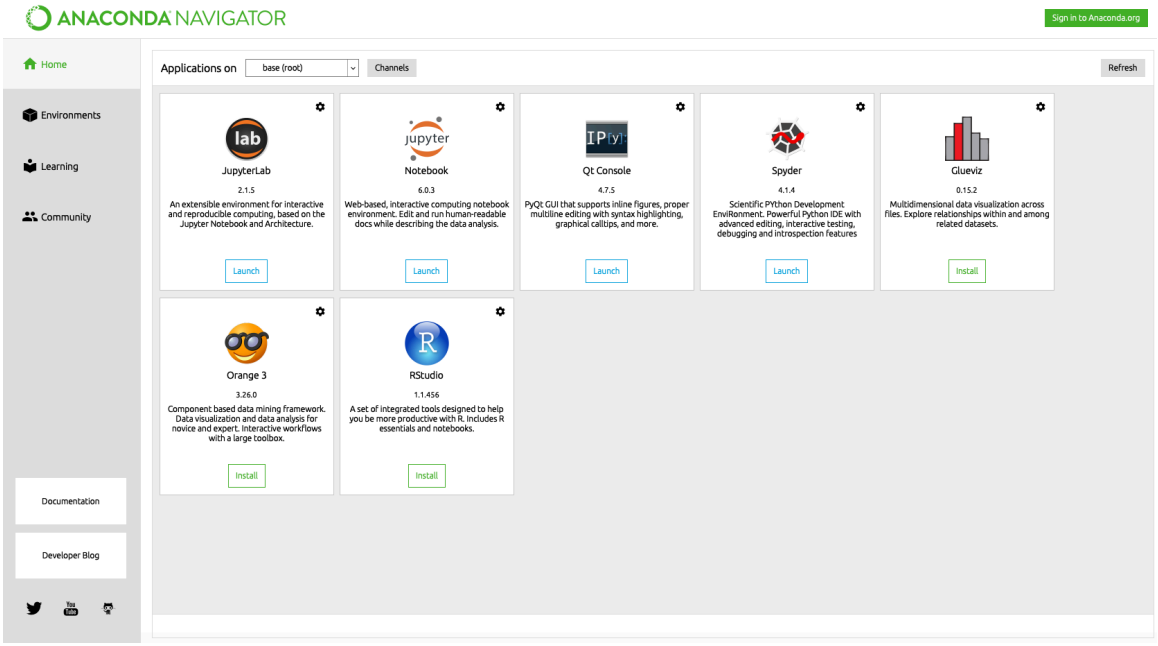
Getting Started with Jupyter Notebook and the Atomic Simulation Environment

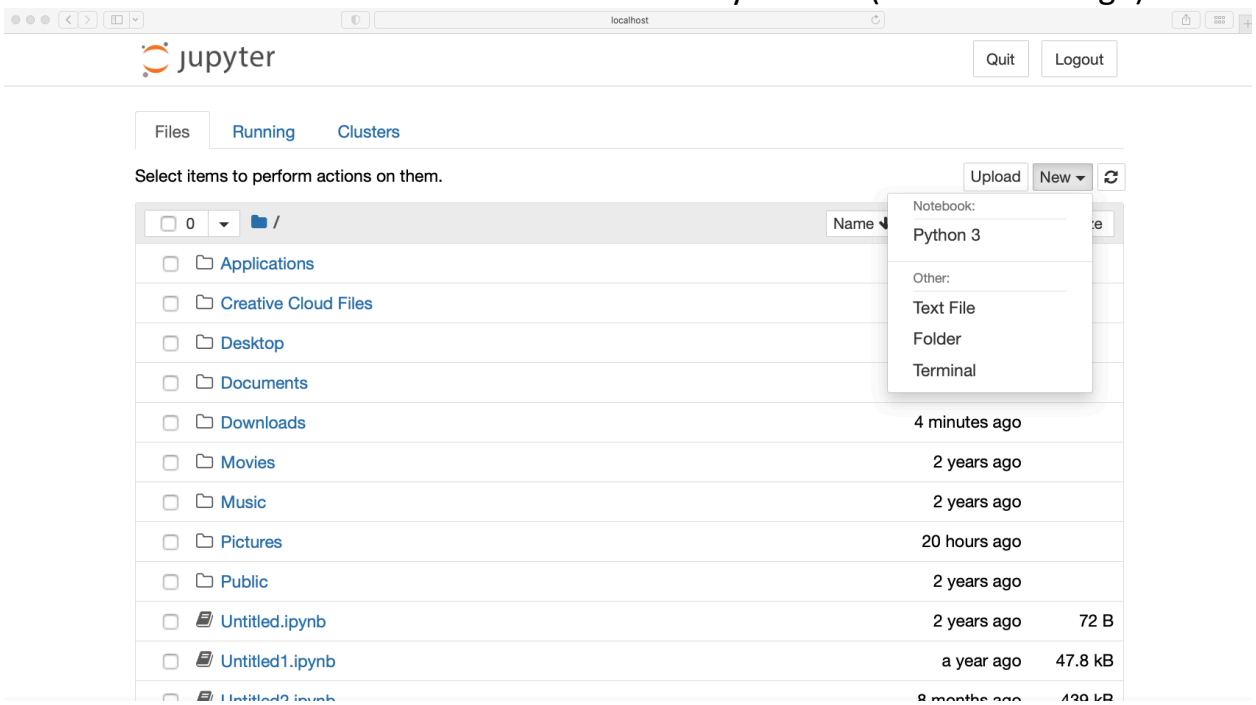
1. Installing Python and Jupyter Notebook:
   If you do not have python and Jupyter Notebook installed, navigate to https://www.anaconda.com/ and follow the download prompts for your OS.



2. Launch **Anaconda Navigator** from your start menu or applications folder. Launch Jupyter Notebook.

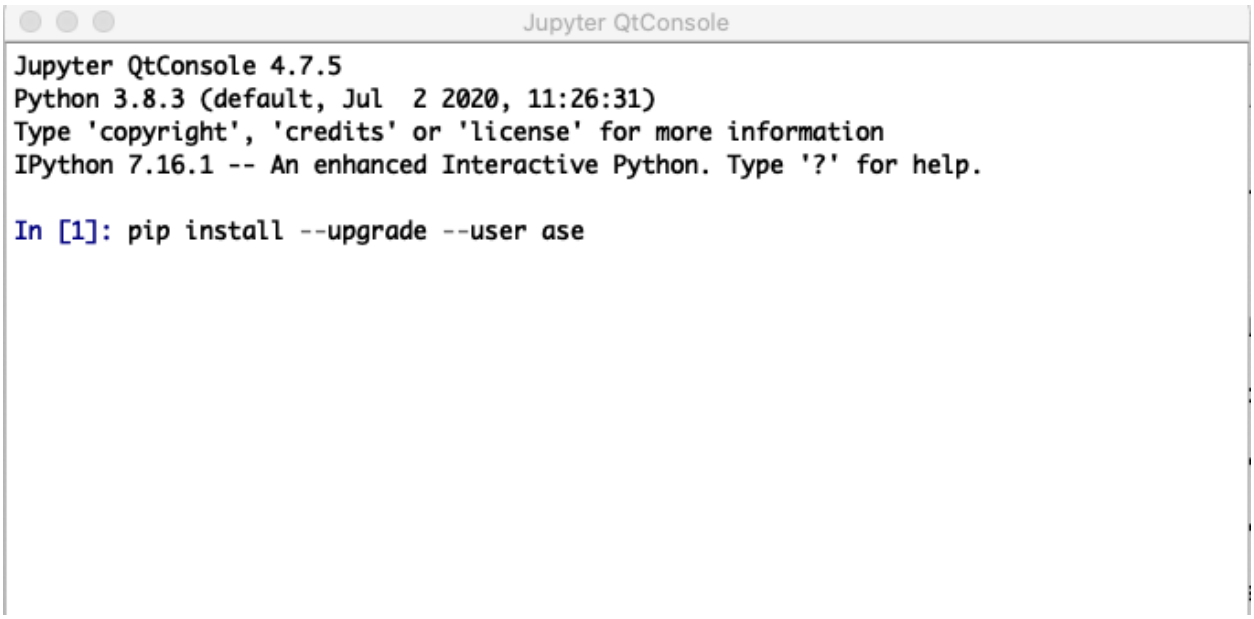


3. A browser window should open with the starting screen for Jupyter Notebook. From this screen select “New -> Python 3” (see below image).

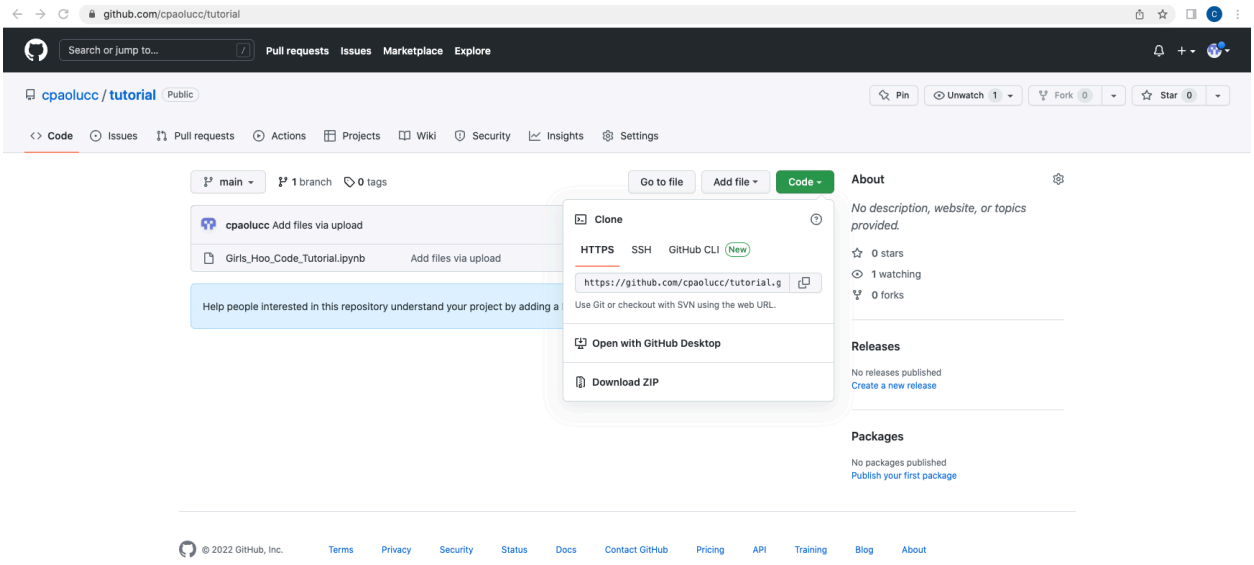


After creating the blank notebook I will give a brief demonstration of coding with python in it.

4. Next, we need to install the Atomic Simulation Environment (ASE) python package, which is not included with the default Anaconda python distribution. Go back to Anaconda and launch the “Qt Console”. Then use the following command in it:
   pip install --upgrade --user ase

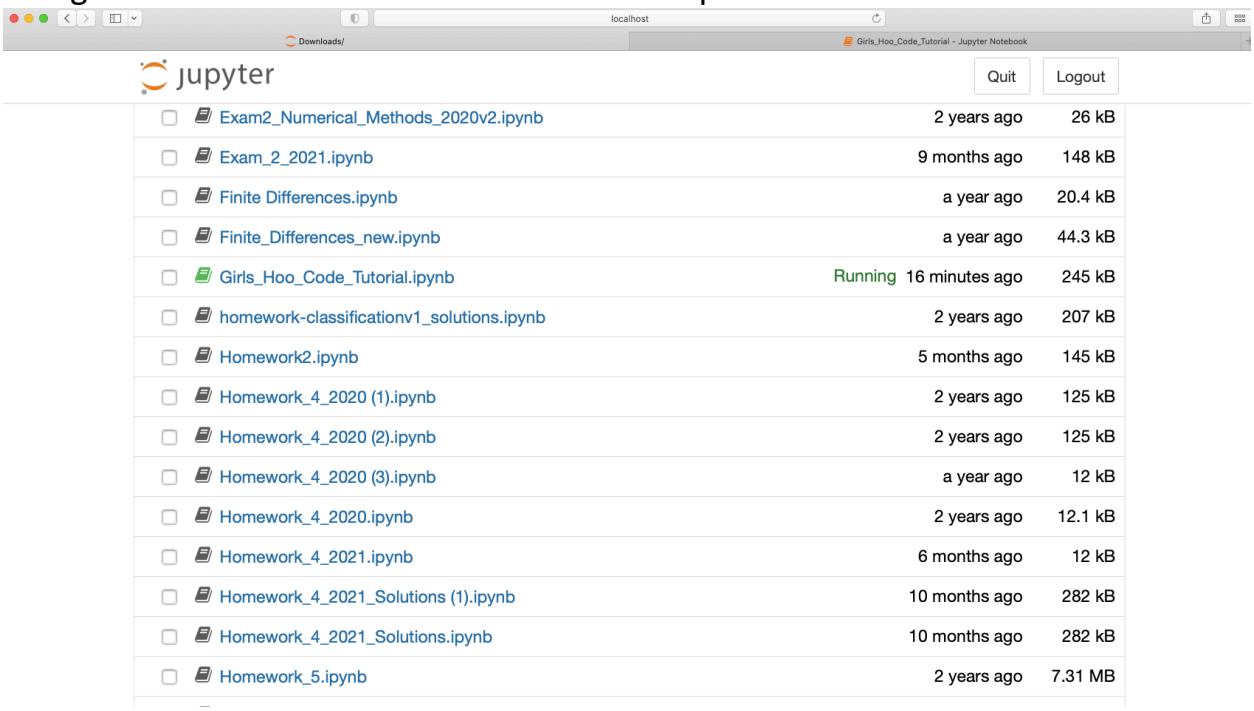


5. Ok, you now have all the components installed to run today’s tutorial! Download the tutorial file and from my Github: https://github.com/cpaolucc/tutorial

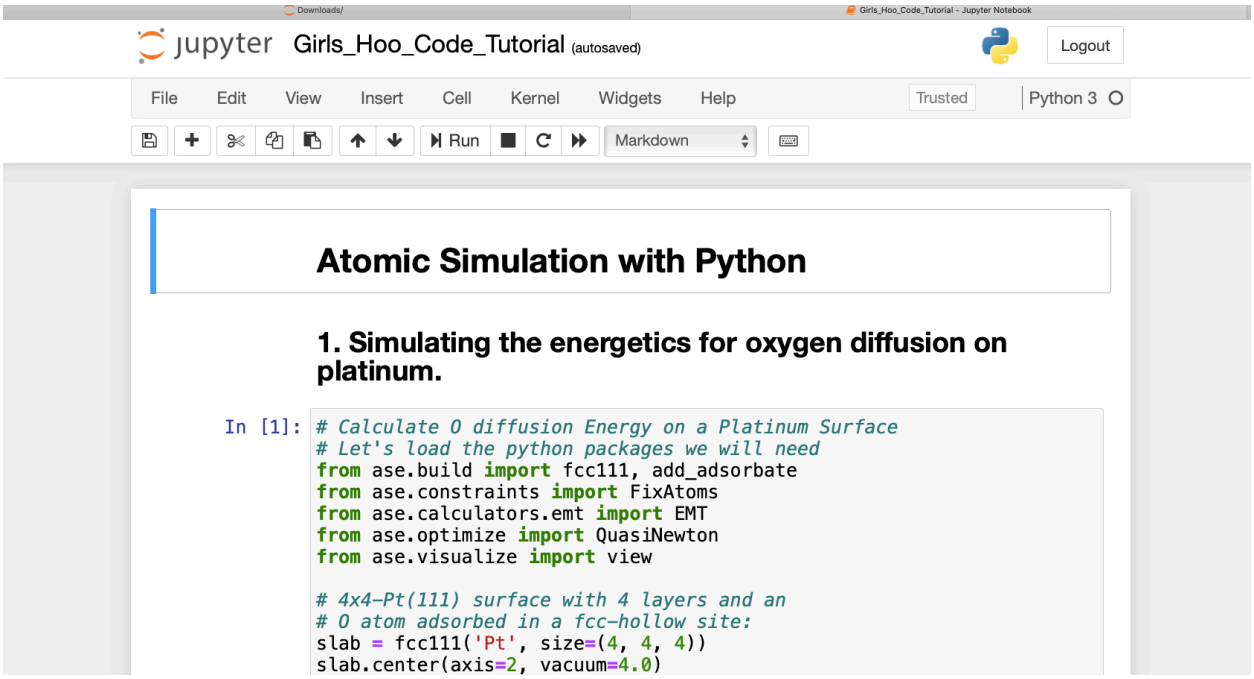


You will need to extract the zip file.

6. You can now go back to the first tab in your browser for Jupyter Notebook. Navigate to the tutorial file and click on it to open.



7. You should now see the following screen:


Downloads/
Girls_Hoo_Code_Tutorial - Jupyter Notebook
jupyter Girls_Hoo_Code_Tutorial (autosaved)
Logout
File Edit View Insert Cell Kernel Widgets Help
Trusted
Python 3
Run
Markdown
Atomic Simulation with Python
1. Simulating the energetics for oxygen diffusion on platinum.
In [1]:
# Calculate O diffusion Energy on a Platinum Surface
# Let's load the python packages we will need
from ase.build import fcc111, add_adsorbate
from ase.constraints import FixAtoms
from ase.calculators.emt import EMT
from ase.optimize import QuasiNewton
from ase.visualize import view
# 4x4-Pt(111) surface with 4 layers and an
# O atom adsorbed in a fcc-hollow site:
slab = fcc111('Pt', size=(4, 4, 4))
slab.center(axis=2, vacuum=4.0)