

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.

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Anaconda offers the easiest way to perform Python/R data science and machine learning on a single machine. Start working with thousands of open-source packages and libraries today.

Download 

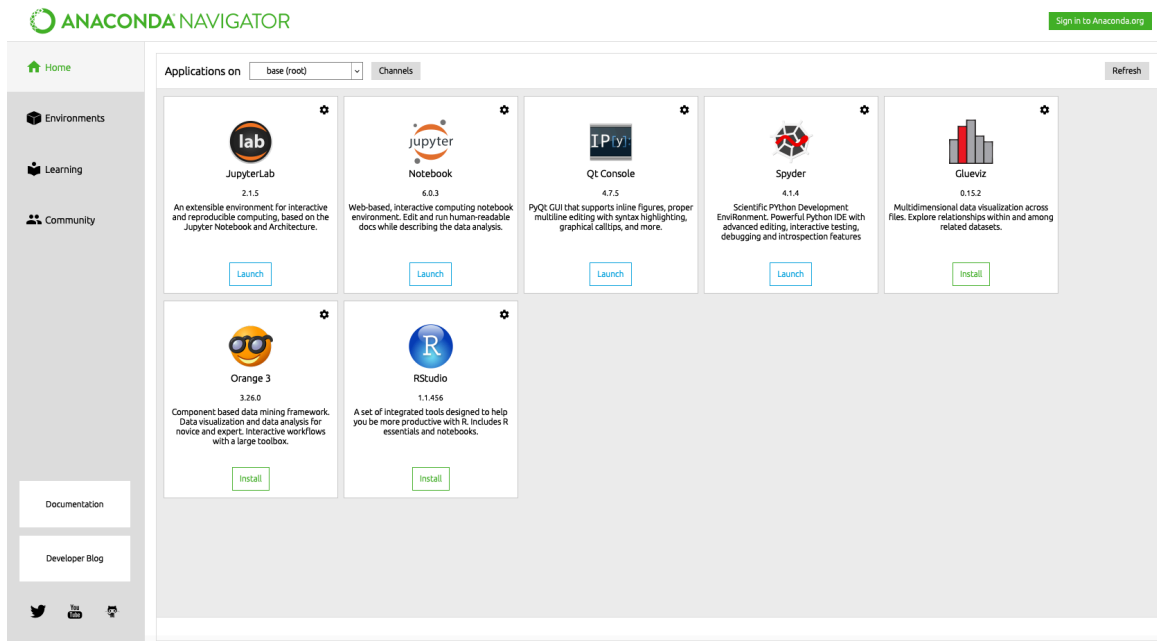
For MacOS

Python 3.9 • 64-Bit Graphical Installer • 591 MB

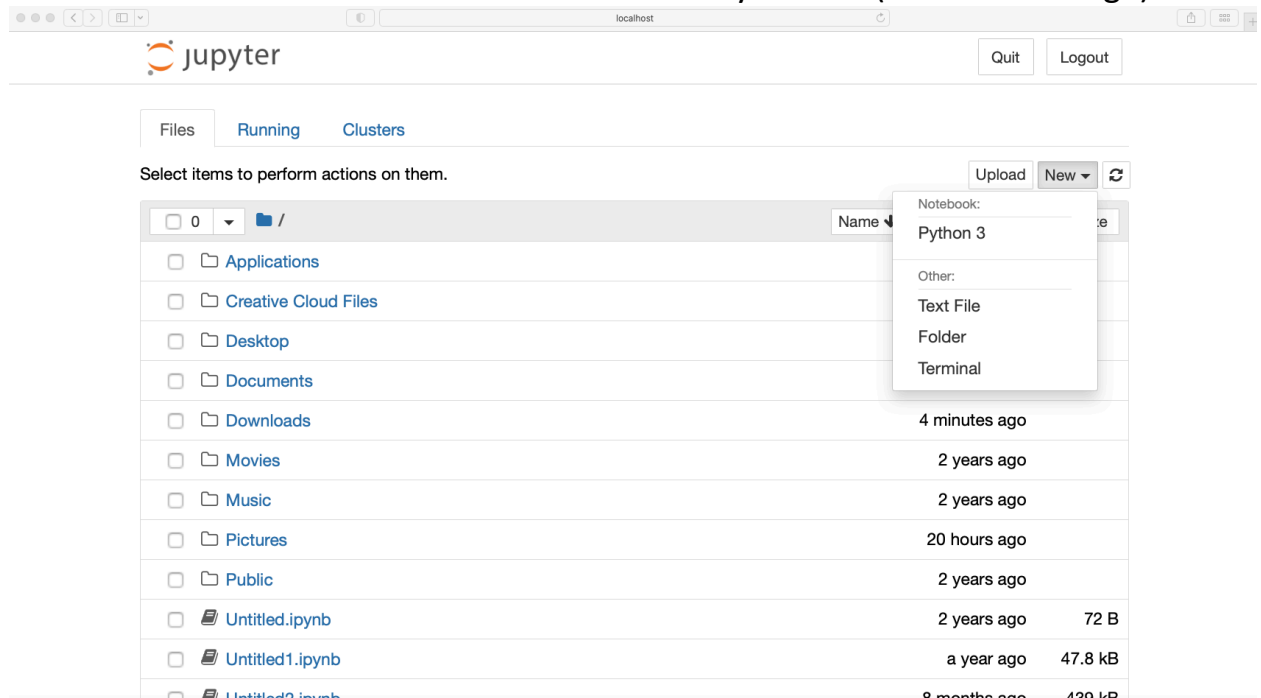
Get Additional Installers



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



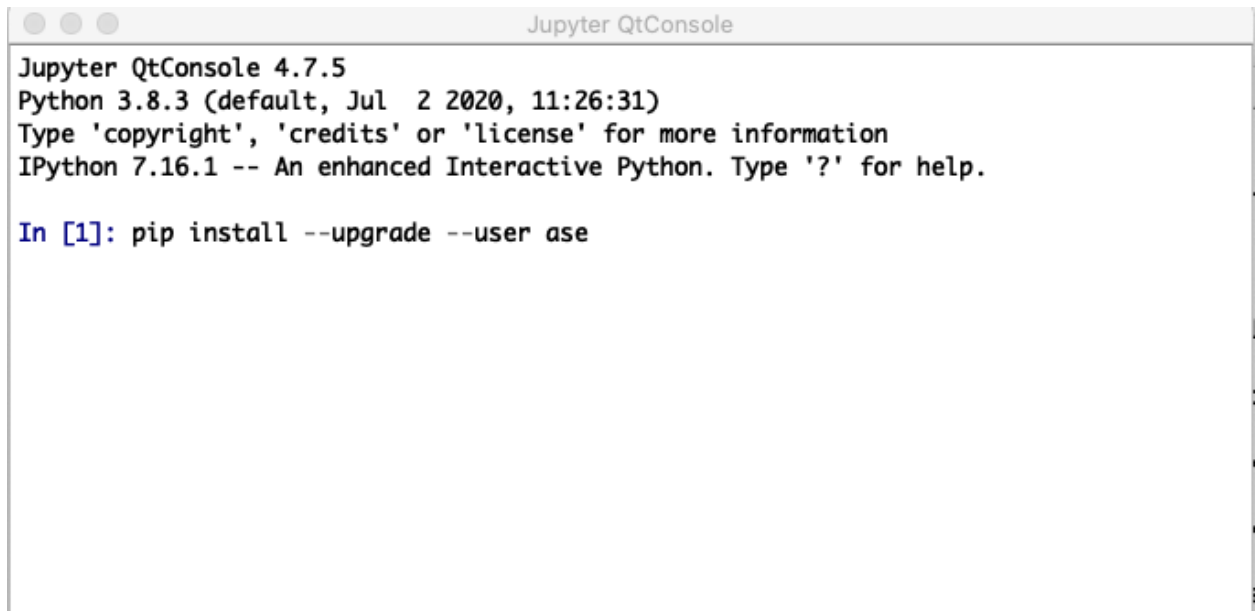
3. A browser window should open with the starting screen for Jupyter Notebook. From this screen select “New -> Python 3” (see below image).



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`

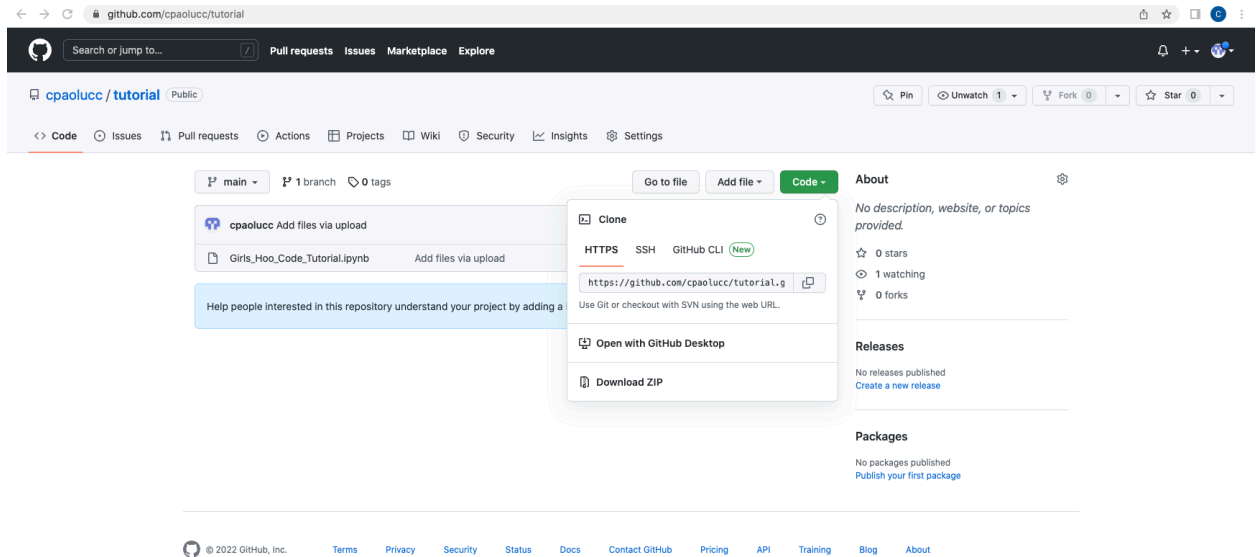


The screenshot shows a window titled "Jupyter QtConsole". Inside the window, the following text is displayed:

```
Jupyter QtConsole 4.7.5
Python 3.8.3 (default, Jul 2 2020, 11:26:31)
Type 'copyright', 'credits' or 'license' for more information
IPython 7.16.1 -- An enhanced Interactive Python. Type '?' for help.

In [1]: 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.

File Name	Last Modified	Size
<input type="checkbox"/> Exam2_Numerical_Methods_2020v2.ipynb	2 years ago	26 kB
<input type="checkbox"/> Exam_2_2021.ipynb	9 months ago	148 kB
<input type="checkbox"/> Finite Differences.ipynb	a year ago	20.4 kB
<input type="checkbox"/> Finite_Differences_new.ipynb	a year ago	44.3 kB
<input type="checkbox"/> Girls_Hoo_Code_Tutorial.ipynb	Running 16 minutes ago	245 kB
<input type="checkbox"/> homework-classificationv1_solutions.ipynb	2 years ago	207 kB
<input type="checkbox"/> Homework2.ipynb	5 months ago	145 kB
<input type="checkbox"/> Homework_4_2020 (1).ipynb	2 years ago	125 kB
<input type="checkbox"/> Homework_4_2020 (2).ipynb	2 years ago	125 kB
<input type="checkbox"/> Homework_4_2020 (3).ipynb	a year ago	12 kB
<input type="checkbox"/> Homework_4_2020.ipynb	2 years ago	12.1 kB
<input type="checkbox"/> Homework_4_2021.ipynb	6 months ago	12 kB
<input type="checkbox"/> Homework_4_2021_Solutions (1).ipynb	10 months ago	282 kB
<input type="checkbox"/> Homework_4_2021_Solutions.ipynb	10 months ago	282 kB
<input type="checkbox"/> Homework_5.ipynb	2 years ago	7.31 MB

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

Atomic Simulation with Python

1. Simulating the energetics for oxygen diffusion on platinum.

```
In [1]: # Calculate 0 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
# 0 atom adsorbed in a fcc-hollow site:
slab = fcc111('Pt', size=(4, 4, 4))
slab.center(axis=2, vacuum=4.0)
```