<u>Software requirements for 7/12/2019 Transition Interface Sampling and Forward Flux Sampling (Sarupria)</u> Github repository: https://github.com/SarupriaGroup/RareEventsSummerSchool2019

The hands-on exercises for this day of the workshop will be delivered through Jupyter notebooks. The Jupyter notebooks use Python 3.6.

You can install Jupyter notebook using Anaconda with Python 3.6: <a href="https://www.anaconda.com/distribution/">https://www.anaconda.com/distribution/</a>

If you have Anaconda installed but not the Jupyter notebooks, you can use conda to install Jupyter notebooks.

conda install jupyter

If you do not have Anaconda you can use pip3 (python package manager) to install Jupyter notebook. pip3 install jupyter

Useful website with instructions:

https://test-jupyter.readthedocs.io/en/rtd-theme/install.html

To start Jupyter notebook:

- Go to the terminal
- Go to the working folder (cd)
- Type jupyter notebook
  - This will open a window in the web browser with the list of available Jupyter notebooks in the folder (see figure below)
- Select the Jupyter notebook you wish to work with

The packages of Python that should be installed for running the codes used in the exercises are:

- numpy
- sys
- math
- random
- matplotlib

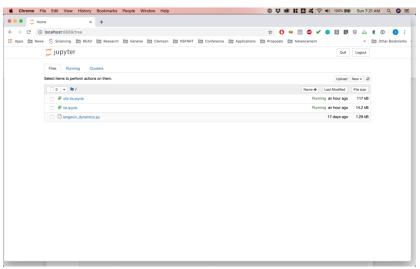


Figure 1: Snapshot of the browser window opened after executing jupyter notebook command