All examples in this tutorial can be run using a Jupter Notebook in the JupyterLab package (<https://jupyter.org/install>). The tutorials require the installation of three python packages:

* ase (<https://wiki.fysik.dtu.dk/ase/install.html>)
* Matplotlib (<https://matplotlib.org/stable/install/index.html>)
* MACE (<https://github.com/ACEsuit/mace>).

The easiest way to install these packages is using the pip python installer. (<https://pip.pypa.io/en/stable/installation/>). Once pip is installed on your system, the necessary packages can be installed using the following procedure:

**In Windows**: Open Windows PowerShell app (or equivalent python environment):

**In Mac OS:** Open Terminal app (or equivalent python environment):

Copy and paste the following lines:

pip install jupyterlab

python -m pip install -U matplotlib

pip install --upgrade ase

pip install mace-torch

To open the Jupyter Notebook ‘mace\_ase\_optimise\_lifepo4.ipynb’, on your computer, type the following in your command terminal:

jupyter-lab mace\_ase\_optimise\_lifepo4.ipynb