Setting up a Conda environment

PUE Advanced Computational Physics
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Some example codes provided for the PUE Advanced Computational Physics class are written in Python 3. The following guide demonstrates how to set up an environment using Anaconda (https://www.anaconda.com).

1 Linux and macOS

If you know what you are doing, you can install python3, jupyter-notebook, and any additionally required modules using the package manager of your Linux distribution. Alternatively, simply follow the instructions below for a local installation in your home directory.

- Download Anaconda (https://www.anaconda.com/distribution/) for Python 3.7
- Install by running:

  ```
  bash <DOWNLOADED FILE>
  ```

  from your terminal.

  a. A simple install to your own home directory suffices.
  b. Say yes to adding code to .bashrc—unless you know better.
  c. Reload your .bashrc:

     ```
     source ~/.bashrc
     ```

  d. Update your conda install:

     ```
     conda update -n base -c defaults conda
     ```

- Now setup the conda environment:
  a. First create a new environment:

     ```
     conda create -n py37 python=3.7
     ```

  b. Now activate the environment:

```
conda activate py37
```

c. Install the packages required to run the example code:

```
conda install notebook ipykernel matplotlib numpy scipy
```

d. If you want to use the python3 kernel in a jupyter notebook you have to execute the following lines:

```
conda install notebook ipykernel
ipython kernel install --user
```

e. You are now good to go—you can either work directly in the environment you just set up or launch a Jupyter notebook using

```
jupyter-notebook
```

f. Once you are done, you can leave the environment by typing

```
conda deactivate
```

2 Windows

- Download Anaconda (https://www.anaconda.com/distribution/) for Python 3.7
- Run the installer, accepting all the defaults. This will install Anaconda to your local directory. Depending on your machine, finalizing the installation might take a long time, but it will finish nonetheless.
- Run *Anaconda Powershell Prompt* from the Windows Start menu.
- Follow the Linux instructions from above, starting at *update your conda install* using

  ```
  conda update -n base -c defaults conda
  ```

- You will have created an entry *Jupyter Notebook (py37)* in your Windows Start menu. You can use this to directly start a Jupyter notebook that uses your newly created environment.

3 Adding modules

- Make sure that you are using the correct environment. Again, you can activate it using

  ```
  conda activate py37
  ```

- Installing an additional package can be as simple as

  ```
  conda install name-of-the-package
  ```

- Many more packages are available at conda-forge:

  ```
  conda install -c conda-forge name-of-the-special-package
  ```