

PROJECT ASSIGNMENT #0: SOFTWARE INSTALLATION

General Information:

- Due date: **Thursday, September 7, 2023 11:59PM**
- Submission on MyCourses
- Cantera can be used with Jupyter Notebook, quite user-friendly, or Spyder, both being Python interfaces. Both are installed using Anaconda. While Spyder offers a similar experience than Matlab, more common to students in general, JN offers a user-friendly interface to write a report.

This first project will ensure that you can install the software, as well as understanding the language used, and solve basic problems.

Part I presents how to install Anaconda, Part II presents how to install Jupyter Notebook, and Part III presents how to install Spyder. Do one or the other, or both if you want to compare them before choosing which one you prefer.

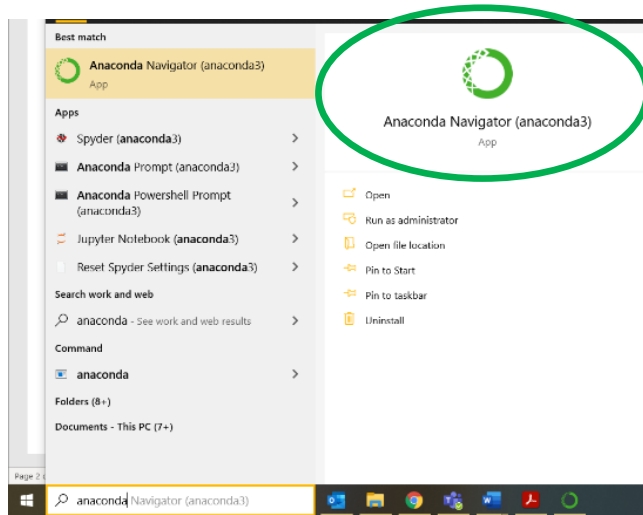
Part IV presents what you need to hand out for this assignment.

Part I – Installation of Anaconda

The installation of Jupyter Notebook and Spyder is done through the installation of Anaconda: <https://www.anaconda.com/products/individual>

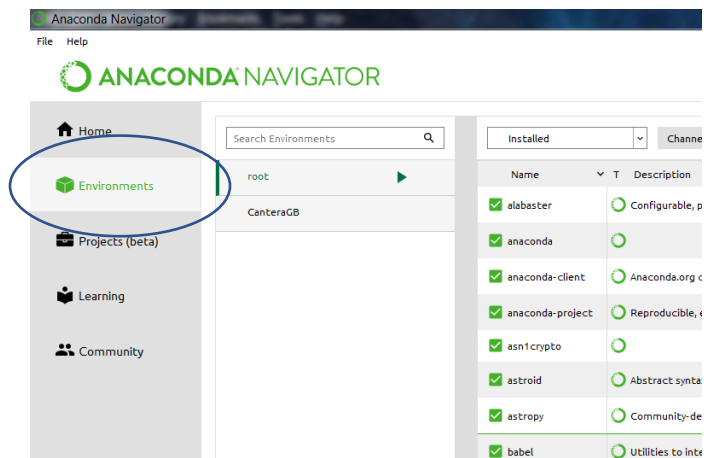
Scroll down the page to select the installer for your operating system; Windows, MacOS, Linux. Select **Python 3.11** 64 bits graphical installer.

After the installation is completed, you will have the following **new software installed** on your machine.

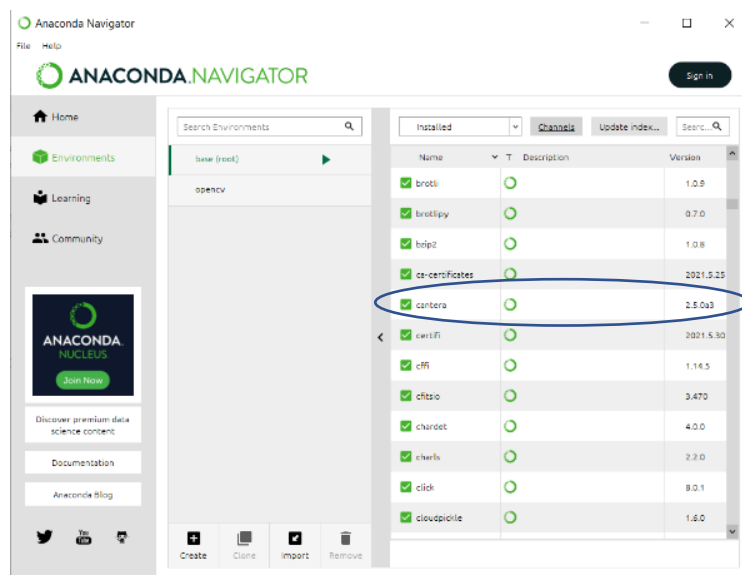


Next you need to start the Anaconda navigator to install Cantera.

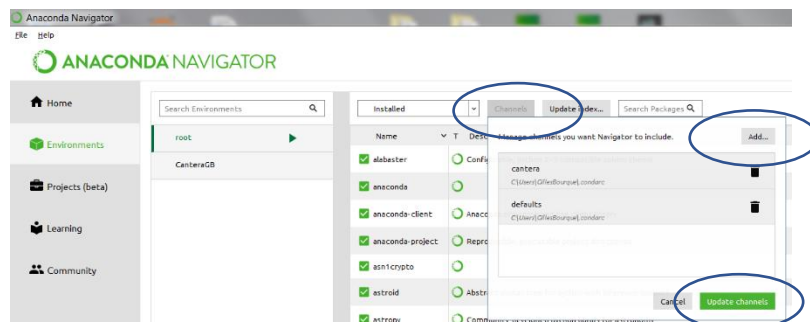
Once Anaconda Navigator is up and running, select the environment tab on the left menu bar:



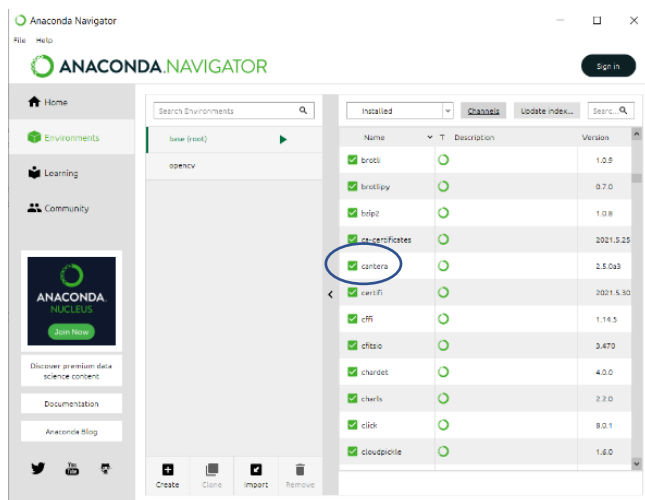
Search for cantera package in the list. If you can't find it, press the Channel button on the top right menu bar:



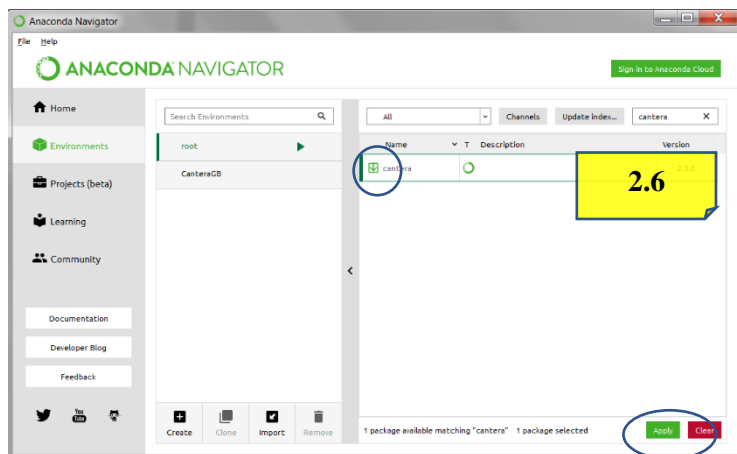
A pop-up window will open as shown above. Click on the Add button and type **cantera** to add a new channel to download Cantera and click Update channel to activate the new channel. Search cantera in the list again to check it is installed.



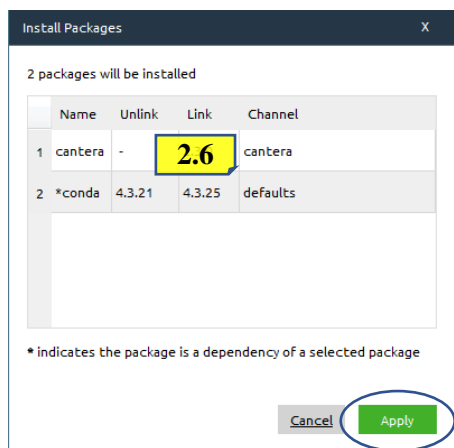
Check the box on the left of the name of the package.



You can now press Apply button at the bottom right of the window.



A pop-up appears and you just need to press Apply at the bottom right of the file.



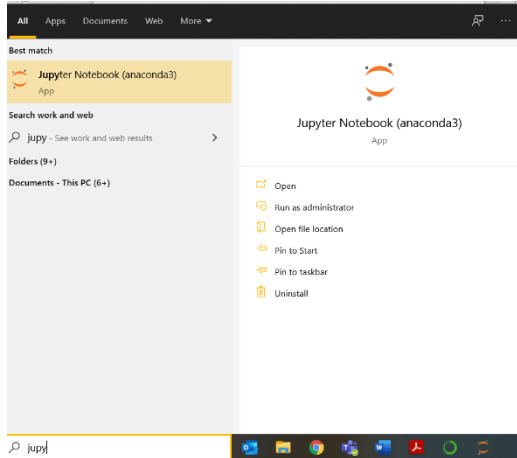
You are now all set and ready to start your first JN.

Part II – Using Jupyter Notebook

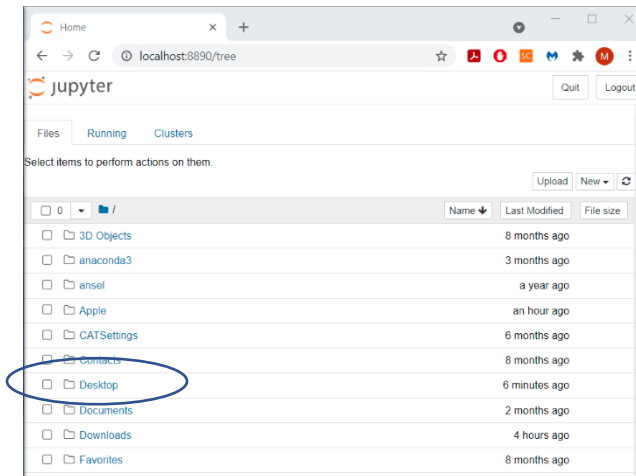
Reminder, use Jupyter Notebook **OR** Spyder, as you wish.

Starting the Jupyter Notebook

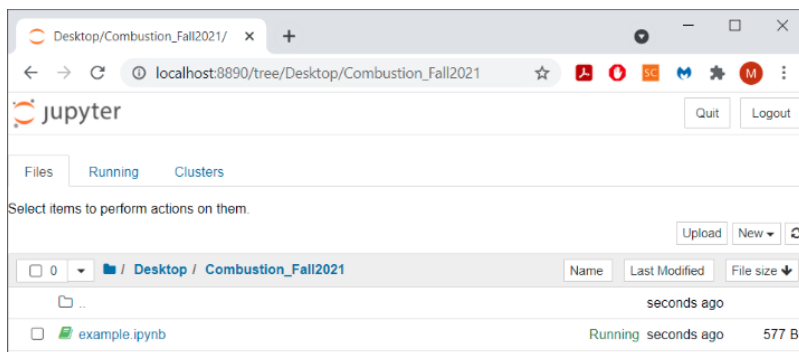
Go back to the main menu and select **Jupyter Notebook**. It is also accessible through the home page of Anaconda.



The kernel will be started in the background and your default browser will open showing the JN interface starting from a default directory. The kernel is the program that communicate between the browser the Python compiler and the operating system. You should see a similar window to this one:

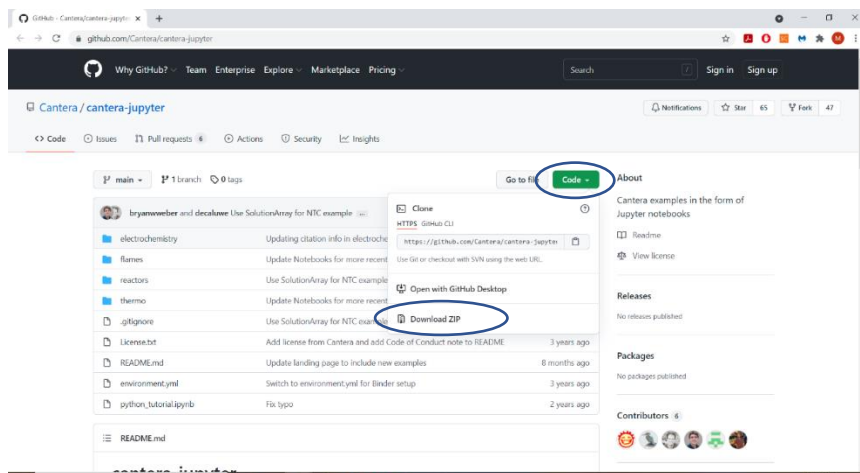


You can see that the folders are the same than the ones from your computer. You can use the desktop as a reference to navigate to the folder of your interest. I strongly advise you to have a specific folder for combustion assignments, directly saved on your disk, and not on an external drive.

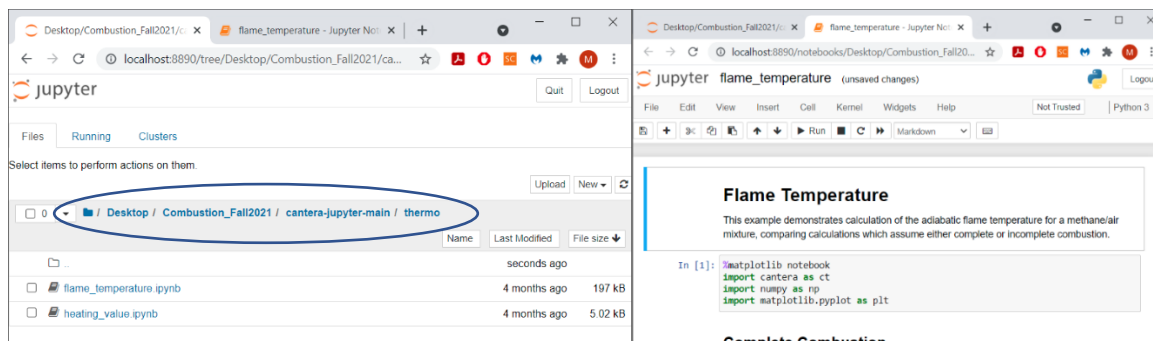


Many Jupyter Notebook are available on the web. For example, go to the github directory of the Cantera for many examples in JN format: <https://github.com/Cantera/cantera-jupyter>

To download the JN to your computer, press the green button, you can clone or download all the files in one go. The file will be saved on your computer in a zip file. Extract the files to a folder of your choice.



Once extracted, use the Jupyter Notebook interface to navigate to this folder. For example, go to the Thermo sub-folder and then select “Flame_Temperature.ipynb” file by double clicking on it. A new tab will display the content of the file.



To learn how to use this webpage as an editor for Python language, **consult** the files *ipython_basics.ipynb*, *Python_Summary.ipynb*, *ipython_matplotlib* on MyCourse and the references below [3-4, 7-8]. A complete book on Python can be found online in different format: Jupyter, pdf, epub, ... [6] and the official Python website [9]. A LaTeX cheat sheet can be found at [11-12].

You will note that all JN files have the extension “.ipynb”.

Getting started with Jupyter Notebook

In order to understand how to code in JN, open the file “P0_Introduction_JN.ipynb” available on MyCourses.

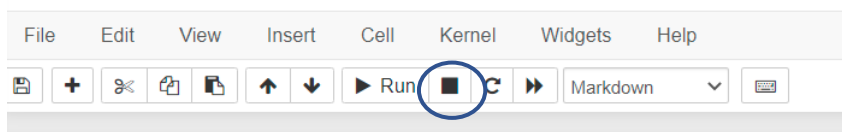
Understand how the file is constructed, how the text is displayed, how to run a cell, how to run the entire document, analyse how the code is written... and **solve** the few problems available in the file.

Some packages are necessary to run your problems smoothly:

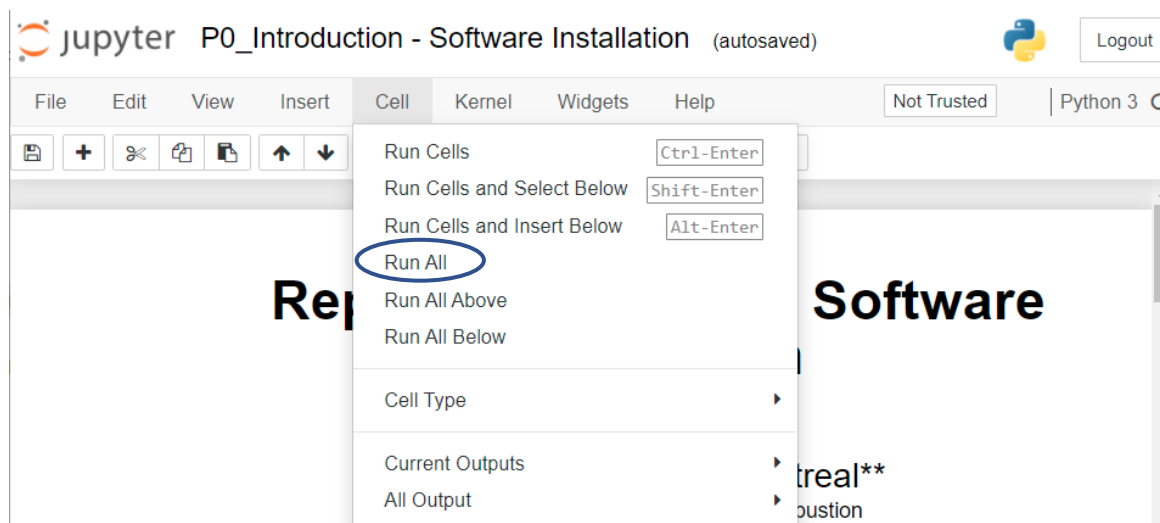
```
%matplotlib inline
import cantera as ct
import numpy as np
import matplotlib.pyplot as plt
```

- The code is working by executing successively the cells of code. Make sure to execute them in the right order, or it could lead to errors.
 - You can check if a cell is executed with the number on the side:
 - No number in bracket = not executed
 - Number in bracket = executed
 - * in bracket = executing, not finished
 - The numbers indicate the order of execution, you can easily check the proper succession of execution
 - An executed cell does not mean that the cell does not have an error!
- Here is a tip to check that your code is working before submission:
 - Stop the code

jupyter P0_Introduction - Software Installation (autosaved)



- Click on Cell, and click on Run all



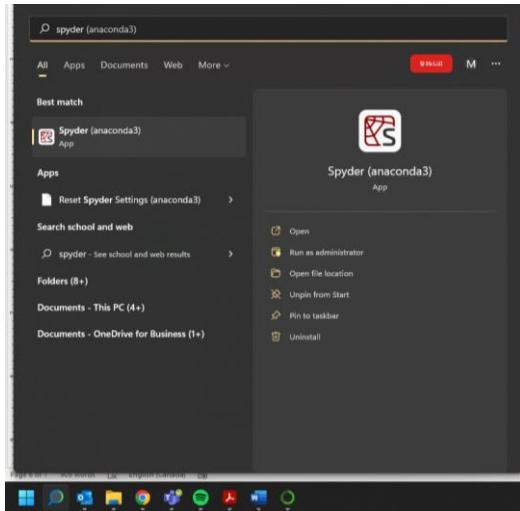
- If there is an error, the cell will display an error, you should fix it, otherwise the following cells won't be executed, unless you execute them by pressing Run all below by positioning your cursor in the cell of interest
- **Save your notebook**
- Extract the graphs and information you need to write your assignment in pdf. **Please, do not include your code!**

Part III – Using Spyder

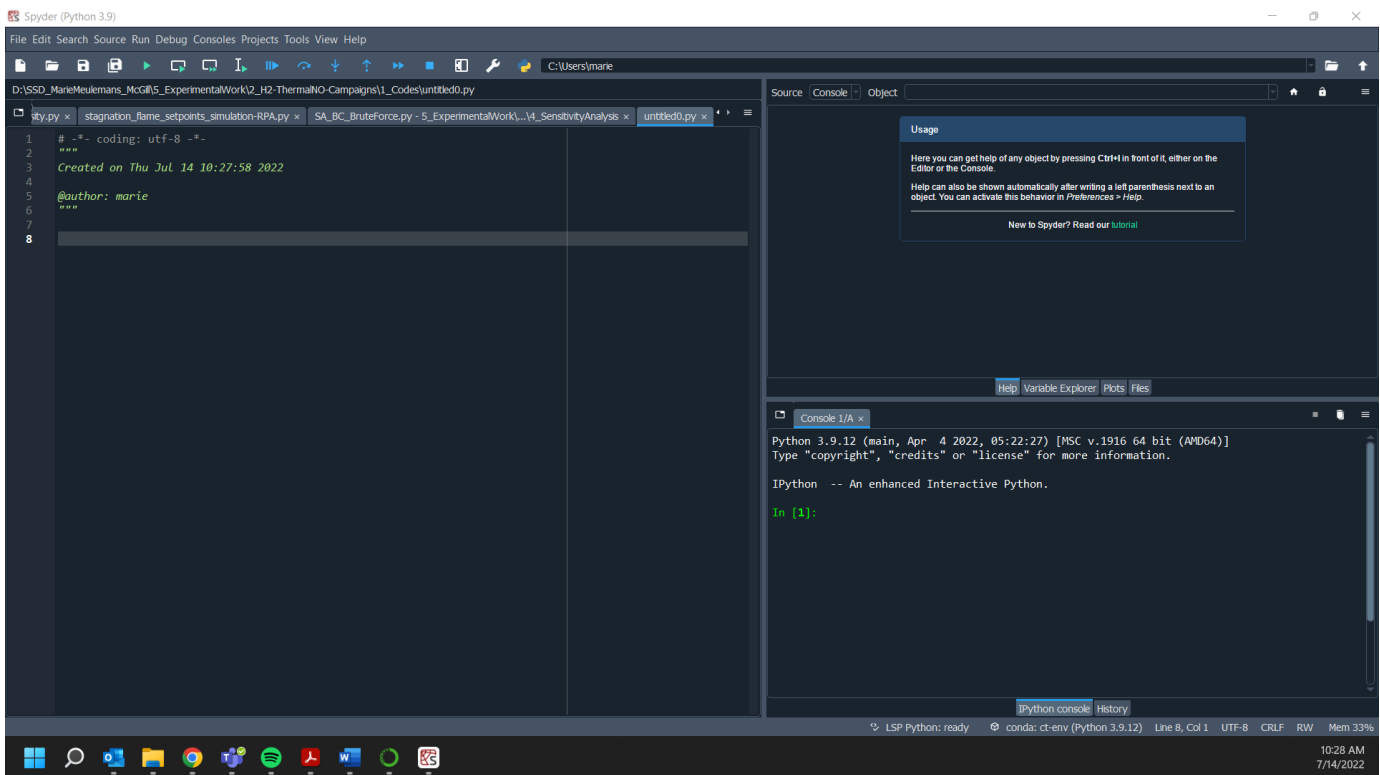
Reminder, use Jupyter Notebook **OR** Spyder, as you wish.

Starting Spyder

Go back to the main menu and select **Spyder**. It is also accessible through the home page of Anaconda.



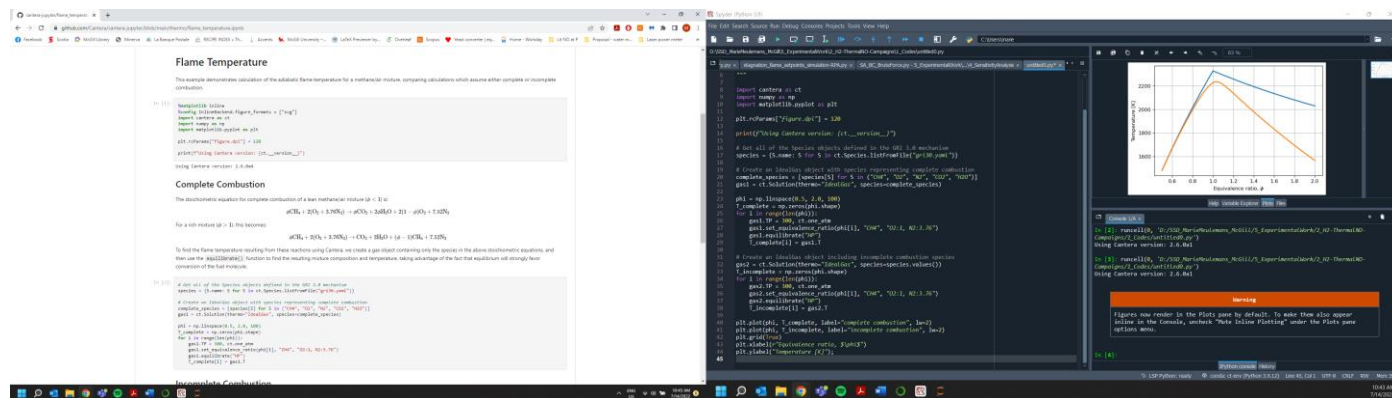
A new untitled project will be started.



On the left is the script. On the top right is the help, variable explorer, and the graph display. On the bottom right is the console.

Make sure to save your script.

Using the following link: https://github.com/Cantera/cantera-jupyter/blob/main/thermo/flame_temperature.ipynb, copy and paste the code (only the code you see in grey cells) in your first script and process it.



You can see that the transition from a JN to Spyder and inversely is very easy.

While Spyder offers a similar experience than Matlab, more common to students in general, JN offers a user-friendly interface to write a report.

Getting started with Spyder

In order to understand how to code in Spyder, open the file “P0_Introduction_Spyder.py” available on MyCourses.

Some packages are necessary to run your problems smoothly:

```
7
8 import cantera as ct
9 import numpy as np
10 import matplotlib.pyplot as plt
11
```

But some are only specific to JN, so do not copy the following:

```
%matplotlib inline
```

- Simply copy the code in grey cells, and execute it.
- If there is an error in the code, it will be displayed in the console.
- **Save your notebook**
- Extract the graphs and information you need to write your assignment in pdf. **Please, do not include your code!**

Part IV – Exercises

For this assignment, solve the few exercises present in the file “P0_Introduction_Spyder.py” or “P0_Introduction_JN.ipynb” available on MyCourses.

Answer the following questions, following the instructions present in the file cited above.

1. What is the version of Python you are using?
2. Present the plot of a sin wave
3. What is the version of Cantera you are using?
4. What is the equilibrium temperature of the methane-air mixture specified?
5. What was the error to correct in the code?
6. Present the plot of a sin wave and cos wave on the same graph
7. What is the command to write to know all the possible objects of a function?

Write your answer in the word processor of your choice, and upload it as a pdf file in MyCourses. **Don’t forget to include your name and your McGill ID number.**

Name your file as follow: *ProjectNumber_FullName_McGillNumber.pdf*

For example: *P0_JohnSmith_0123456789.pdf*

References

Cantera

1. <https://github.com/Cantera/cantera> Github website
2. <http://cantera.github.io/docs/sphinx/html/cython/tutorial.html> Python interface Tutorial

Jupyter Notebook, IPython, Python, Matplotlib and LaTeX

3. <http://jupyter-notebook.readthedocs.io/en/latest/examples/> Jupyter Documentation
4. <http://ipython.readthedocs.io/en/stable/> IPython Documentation
5. [http://nbviewer.jupyter.org/github/ipython/ipython/blob/4.0.x/examples/IPython Kernel/Plotting in the Notebook.ipynb](http://nbviewer.jupyter.org/github/ipython/ipython/blob/4.0.x/examples/IPython%20Kernel/Plotting%20in%20the%20Notebook.ipynb) Matplotlib Tutorial.
6. <http://greenteapress.com/wp/think-python/> A free book on Python
7. <http://maxmelnick.com/python-beginner-tips-and-tricks.html> Jupyter summary
8. https://github.com/maxmelnick/jupyter_keyboard_shortcuts_snippets Practice JN
9. <https://www.python.org/> Python Documentation
10. <http://hplgit.github.io/bumpy/doc/pub/sphinx-basics/index.html> A very basic introduction to scientific Python programming
11. <https://wch.github.io/latexsheet/> Latex cheat sheet
12. <https://users.dickinson.edu/~richesod/latex/latexcheatsheet.pdf> Latex Cheat sheet