CERFACS

EUROPEAN CENTRE FOR RESEARCH AND ADVANCED TRAINING IN SCIENTIFIC COMPUTING

Cantera

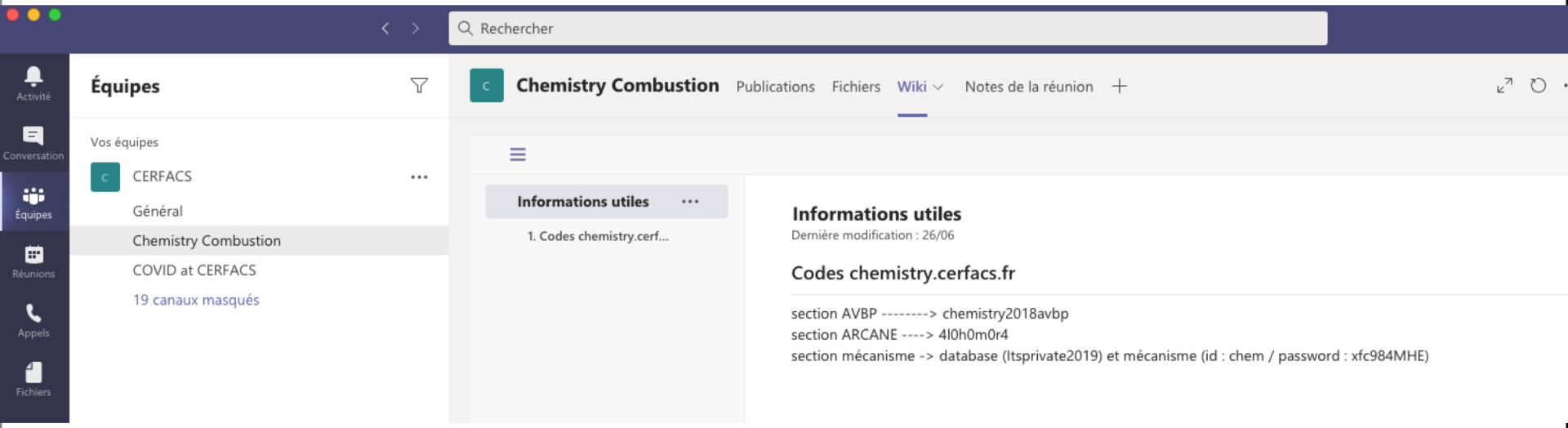
Basics to get started with the tutorial

Tuesday 16th November 2020

www.cerfacs.fr

A word about website and password

To retrieve password on the website, you should go on the teams of chemistry combustion !



Installing CANTERA

The procedure is written on the website.

Two solutions :

- Either you work with your computer, then *git clone* the sources and run the *install_cantera.py*.
- Or you work with NFS, *module load cantera* should be sufficient.

How to work with jupyter notebook (2)

Jupyter python notebook works just like python script, but are more suitable for visualization.

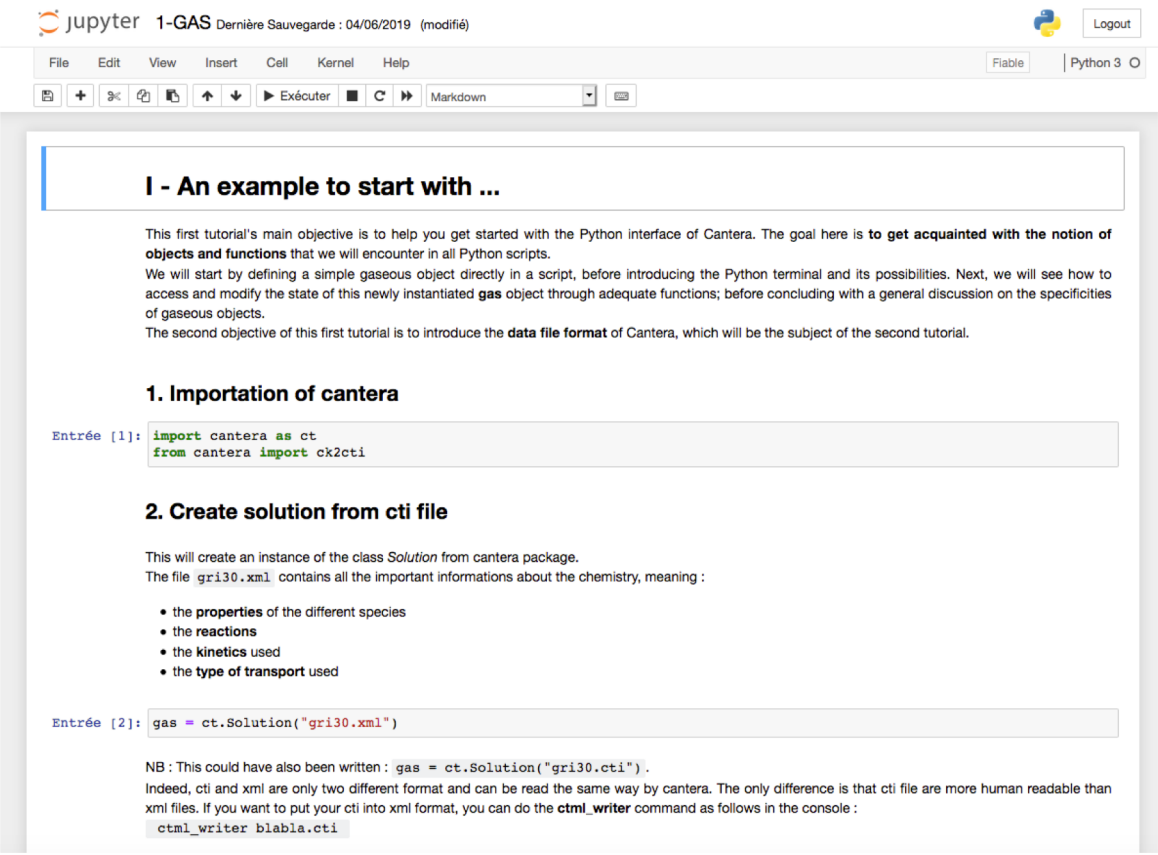
```
jupyter notebook 1-GAS.ipynb
```

If you are on your mac, maybe you have to type :

```
pip3 install --user jupyter
```

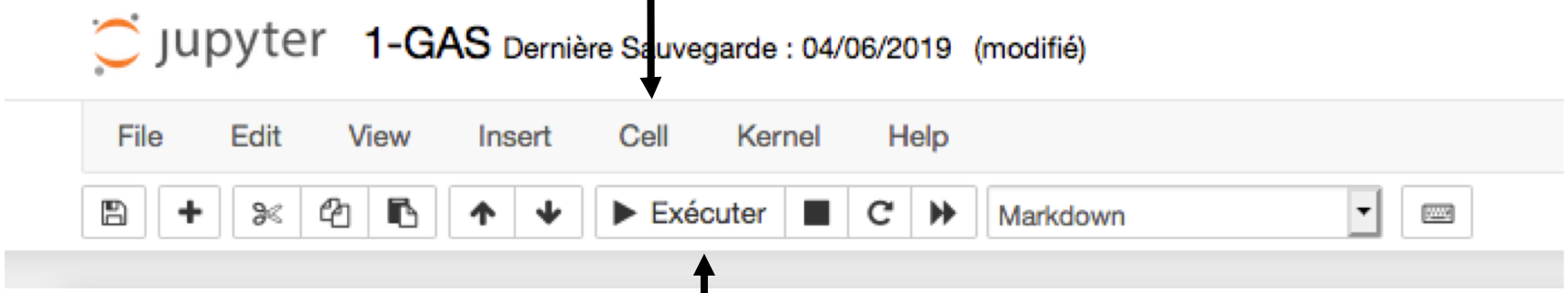
How to work with jupyter notebook

It will open a kernel. Then, a page on your browser will open :



How to work with jupyter notebook

There you can launch all the script



This launches a cell of the script

1. Importation of cantera

This is a markdown cell

Entrée [1]:
```
import cantera as ct
from cantera import ck2cti
```

This is a code cell

2. Create solution from cti file

This will create an instance of the class *Solution* from cantera package.
The file `gri30.xml` contains all the important informations about the chemistry, meaning :

Comments

If you have some comments/feedbacks, do not hesitate to tell us !