Exercise Session 2

IESM Fall 2024-2025

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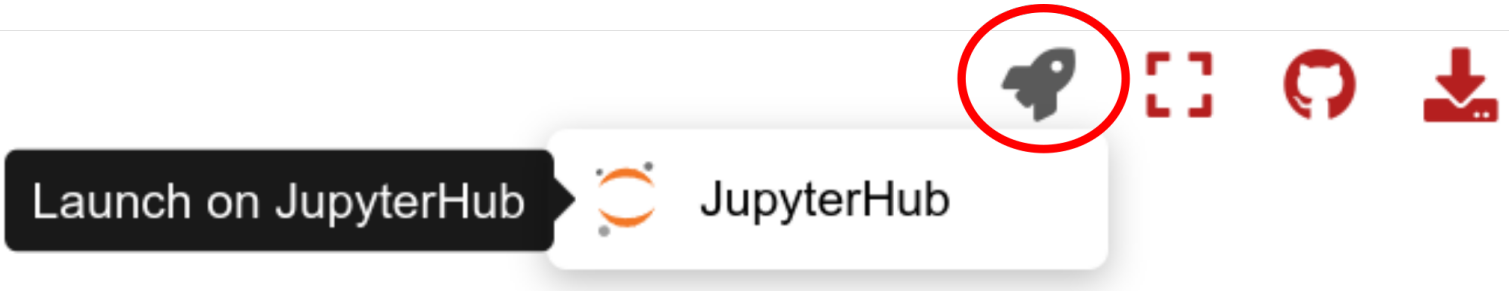
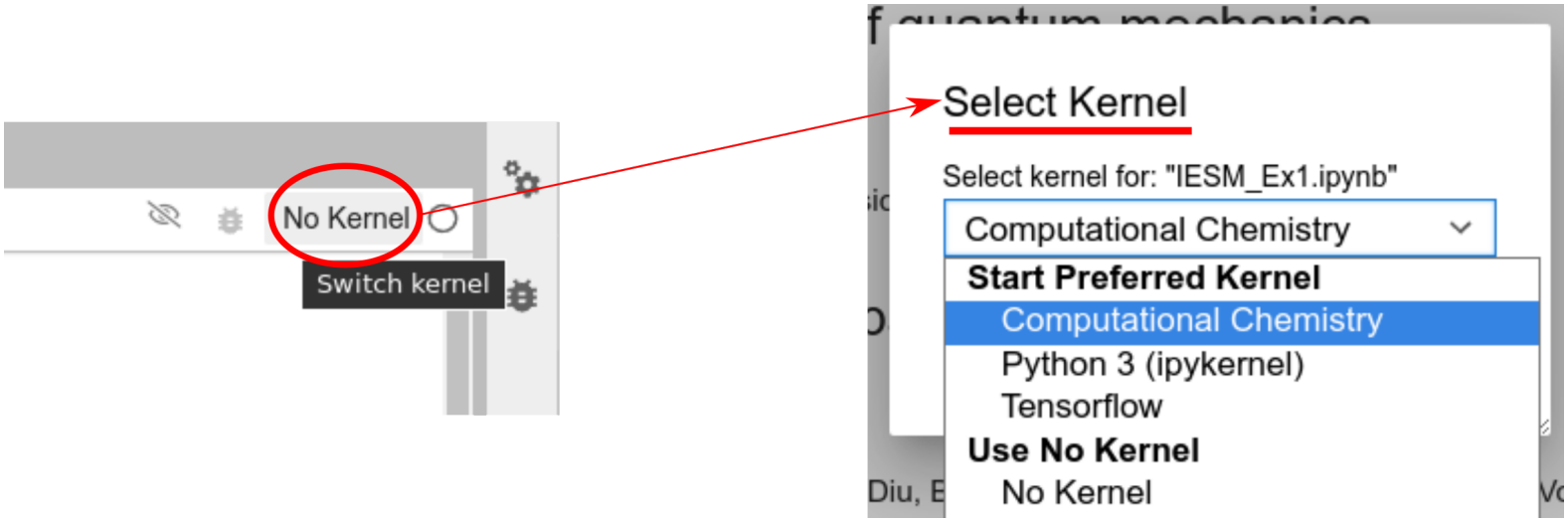
September 24, 2024

Notebook Reminders

- If you're on our exercise website click the rocket button on the top right, choose JupyterHub (noto.epfl.ch)

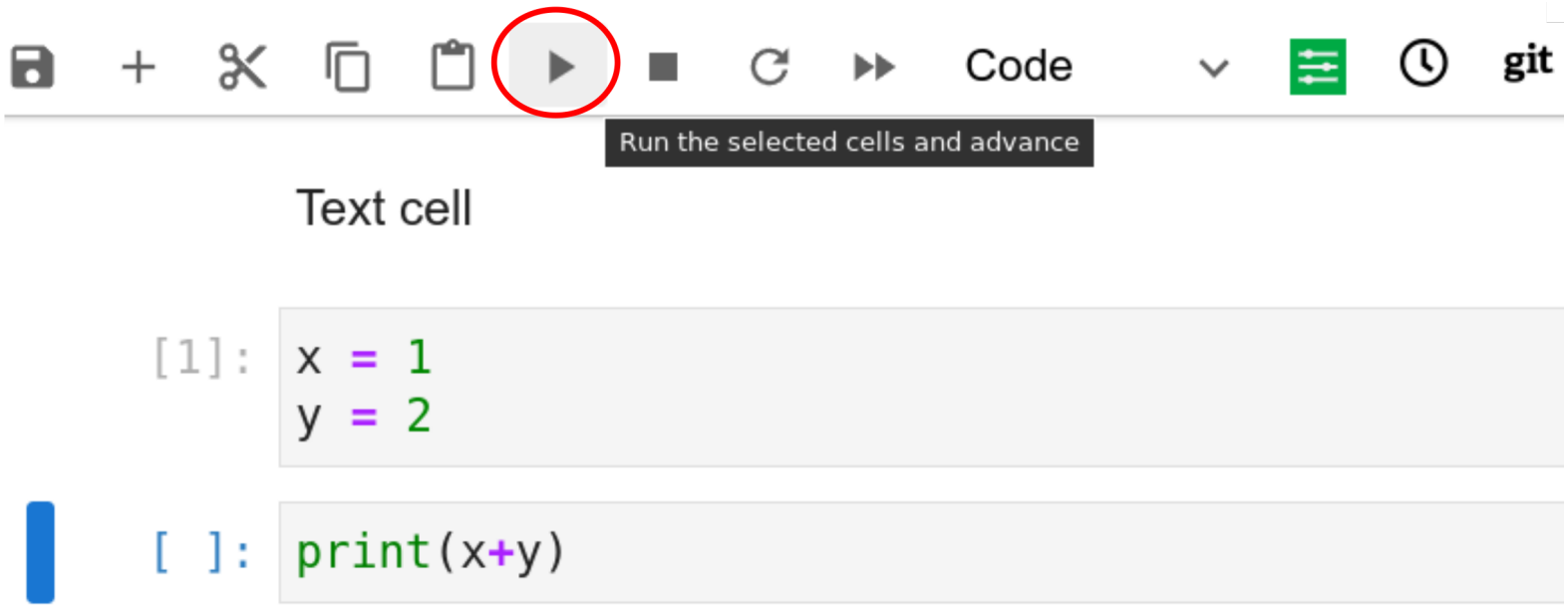


- Make sure to always activate (top right) the `Computational Chemistry` kernel



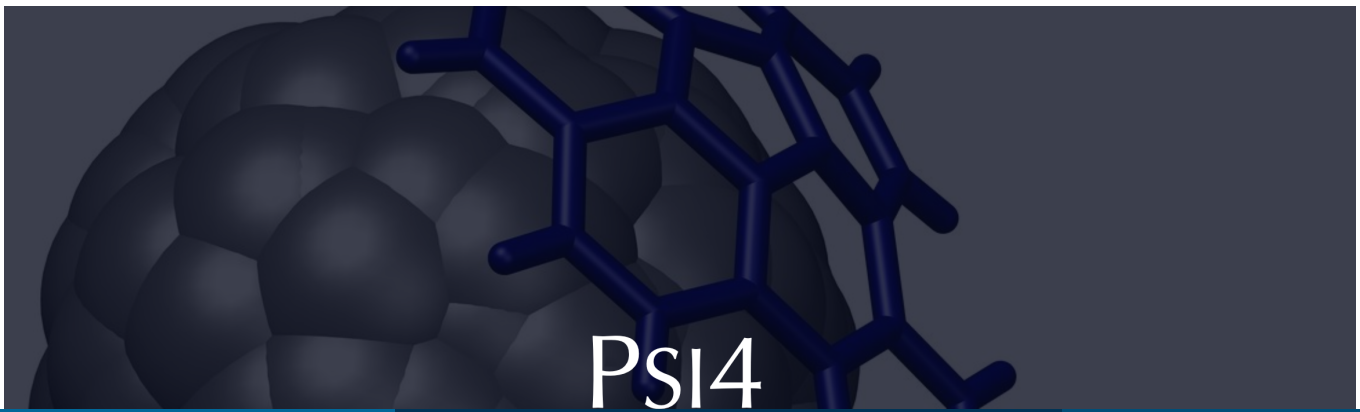
Notebook Reminders

- `.iynb` files organized in cells
  - Markdown (text)
  - Code
- You can edit the cells directly
- Run a code cell by pressing `Play` button (or `Ctrl+Enter` or `Shift+Enter`)



Psi4 Introduction

- Psi4 Manual
- Open-Source ab initio electronic structure software package
- Allows for calculations such as: HF, CI, DFT, molecular energies/structures, reaction mechanisms, transition state search, vibrational frequencies, molecular orbitals/densities, geometry optimization, atomic charges, electrostatic potentials, NMR properties, and more
- Other electronic structure software you may know: Gaussian, CP2K, CPMD, Quantum Espresso, ORCA, NWChem



Psi4 with Python

- We can use Psi4 as a python module with PsiAPI directly in Jupyter Notebooks
- We import Psi4 and use the `psi4` directive to ask Psi4 to perform an action

[1]:
```
import psi4
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt

plt.style.use(['seaborn-poster', 'seaborn-ticks'])
```

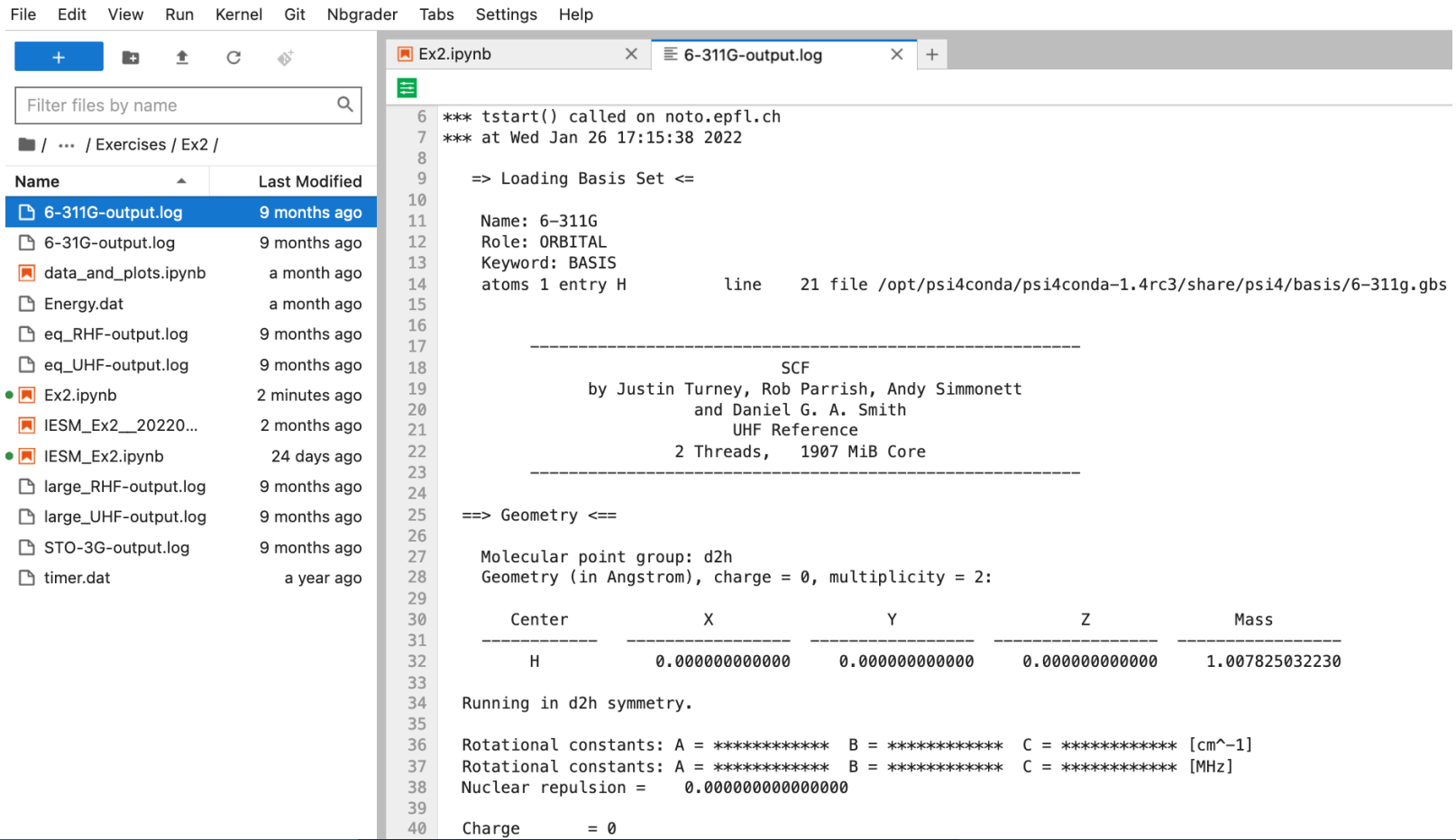
[2]:
```
psi4.set_memory('2 GB')
psi4.set_num_threads(2)
```

```
  Memory set to   1.863 GiB by Python driver.
  Threads set to 2 by Python driver.
```

[3]:
```
h = psi4.geometry("""
0 2
H 0.0 0.0 0.0
""")
```

Viewing Output

- We often set an output file (usually a `.log` file) to store information from a calculation
- You can find them in the lefthand navigation directory



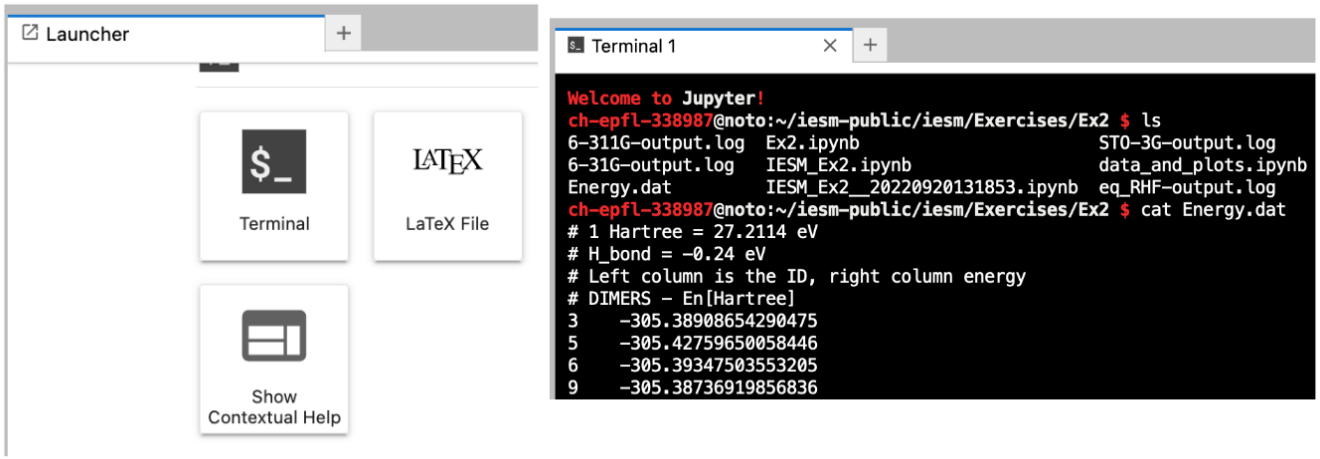
Linux & Terminal

- Linux bash commands in notebooks (cell starts with `!`)

```
!grep 'iter' large_RHF-output.log
```

```
@DF-RHF iter   1:    -0.73775656591694   -7.37757e-01   2.26180e-02 DIIS
@DF-RHF iter   2:    -0.74503745659583   -7.28089e-03   2.27444e-03 DIIS
@DF-RHF iter   3:    -0.74511202947724   -7.45729e-05   5.15094e-06 DIIS
@DF-RHF iter   4:    -0.74511202986000   -3.82762e-10   6.49170e-09 DIIS
```

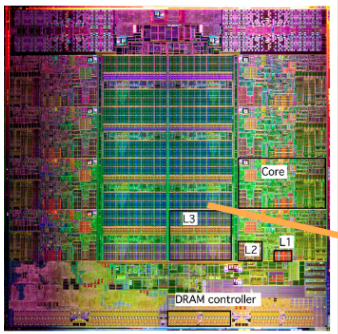
- Linux commands (even Psi4 calculations) directly via a terminal view of your notebooks

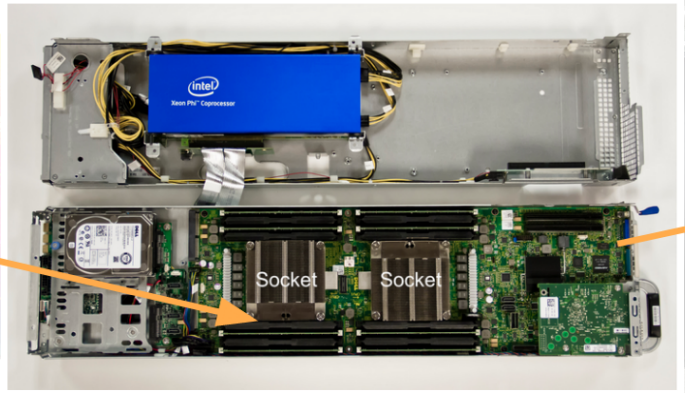


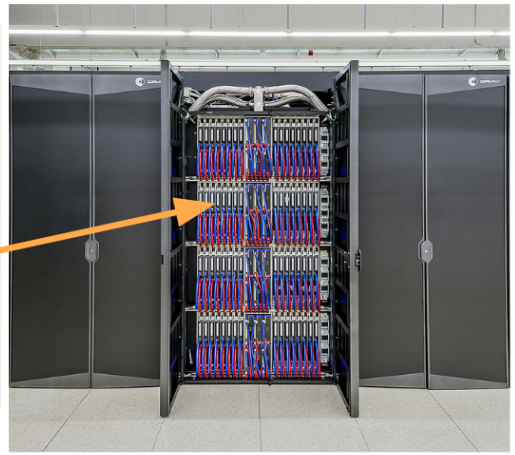
Jupyter Servers

- *"Noto can run up to 15 parallel Jupyter backend servers to provide a total of up to 240 GB of RAM and 240 CPU, shared between all users. Our current policy is to allocate up to a maximum of 2 GB of RAM and 2 CPUs per user."*

Node > Socket > Core (independent processing unit)







Intel Sandybridge socket with eight cores

Stampede node with two sockets and a co-processor

Server room

(Images from TACC HPC textbook)

Exercise 2 - Basis Sets & Psi4

First steps in Psi4 - Exercise page

- Understand what are basis functions
- Get familiar with basis function notation
- Basics of Psi4
- Get familiar with molecular geometries

🎯 Learning goals	📖 Chapter in script	📚 Resources
Understand what are basis functions Get familiar with basis function notation Basics of Psi4 Get familiar with molecular geometries	Chapter 3 - Basis functions in quantum chemistry	Jensen, F. (2017). Introduction to computational chemistry. John wiley & sons. • Chapter 5 - Basis Sets

Exercise 2 - Tips

Tips!

- Please focus on understanding basis sets well first and then getting familiar with Psi4 :)
- Practice single-point calculations for an H-atom and water molecule with `psi4.energy()` commands
  - Requires input geometry (Z-matrix or Cartesian coordinates)
  - Psi4 finds lowest energy combination of wavefunction coefficients for the given geometry
  - By comparing energy values with different basis sets we can discuss the effect of basis set selections on accuracy and cost (Additional note: is the total energy always meaningful? – think about that expecially in the H_2O exercise)
  - We will compute the energy of the system with the selected basis set **and** a method of choice. In this exercise we will always be UHF (unrestricted Hartree Fock), but don't worry too much about it for now: you will get familiar with this and other methods in the next lecutres/exercises!