

# Exercise Session 2 IESM Fall 2024-2025

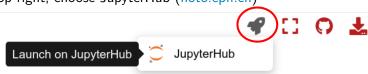
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September 24, 2024

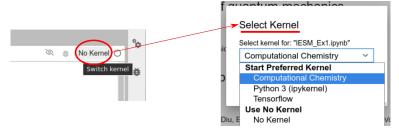


#### Notebook Reminders

 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

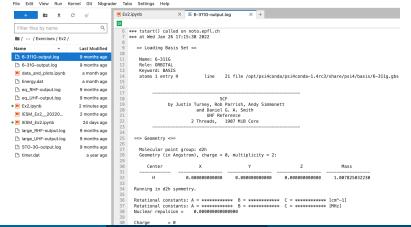
- We can use Psi4 as a python module with PsiAPI directly in Jupyter Notebooks
- We import Psi4 and use the psi4 directive to ask Psi4 to perform an action

```
[1]: import psi4
     import pandas as pd
     import numpy as np
     import matplotlib.pvplot 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("""
     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

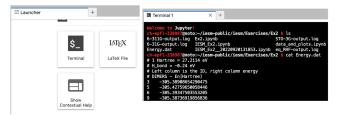
@DF-RHF iter 1: -0.73775656591694 -7.37757e-01 2.26180e-02 DIIS

@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

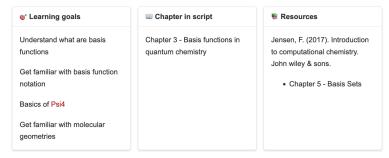
Server room

(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



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## 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<sub>2</sub>O 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!