Exercise Session 2
IESM Fall 2025-2026

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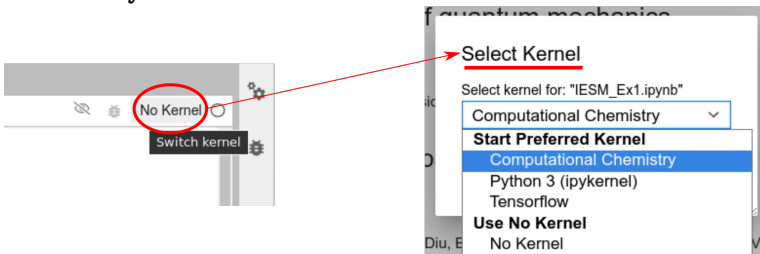
September 23, 2025

- If you're on our exercise website click the rocket button on the top right, choose JupyterHub (noto.epfl.ch)
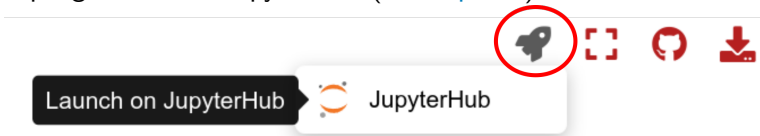
- Make sure to always activate (top right) the Computational Chemistry kernel

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
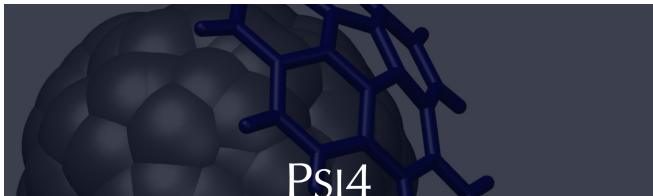
Psi4

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

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

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

```python
[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.
```

```python
[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
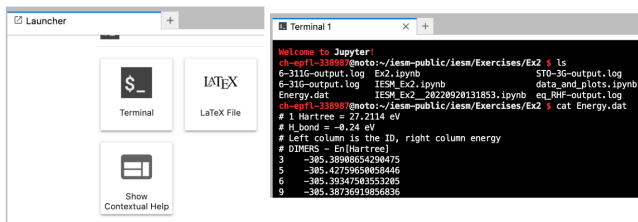
Jupyter Servers

- *"Noto can run up to 20 parallel Jupyter backend servers to provide a total of up to 320 GB of RAM and 320 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)
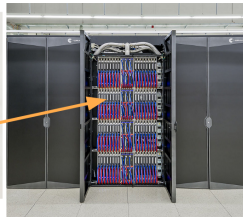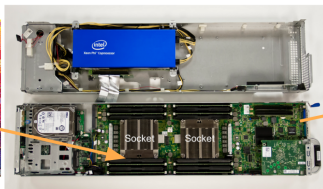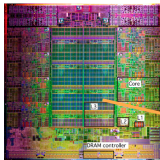
Intel Sandybridge socket with eight cores
Stampede node with two sockets and a co-processor
Server room

(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	Chapter 3 - Basis functions in quantum chemistry	Jensen, F. (2017). Introduction to computational chemistry. John wiley & sons.
Get familiar with basis function notation		Chapter 5 - Basis Sets
Basics of Psi4		
Get familiar with molecular geometries		

Exercise 2 - New exercise questions

New exercise questions!

- The two parts of the exercise on the helium atom (section 2.2.4) and on beryllium hydride (section 2.4) are new.
- Therefore, please let us now if something is unclear in the text, questions or the tasks we ask you to perform :)
- These modifications include questions 9, 13, and 14.
- **Total of 14 questions**
- **Due date for the written report next Tuesday (September 30, 10am)**

Exercise 2 - Tips

Tips!

- Please focus on understanding basis sets well first and then getting familiar with Psi4 :)
- Practice single-point calculations for an single atom and simple 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, here only 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 lectures/exercises!