

Exercise Session 2

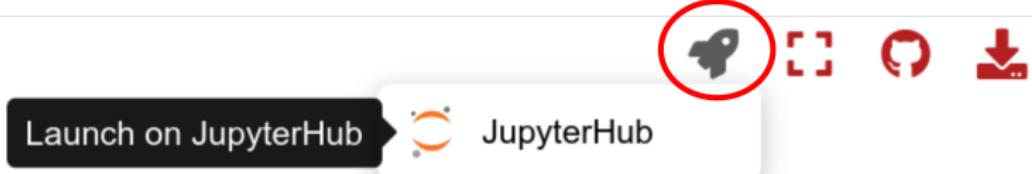
IESM Fall 2025-2026

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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)

The screenshot shows a Jupyter Notebook interface. At the top is a toolbar with various icons: a file icon, a plus sign, a cross, a square, a clipboard, a play button (circled in red), a square with a dot, a circular arrow, a double right arrow, a 'Code' button, a dropdown menu, a green grid, a clock icon, and a 'git' icon. Below the toolbar, a button says 'Run the selected cells and advance'. The main area contains two code cells. The first cell is labeled 'Text cell' and contains the code: [1]: x = 1
y = 2. The second cell is labeled '[]:' and contains the code: print(x+y).

```
[1]: x = 1
      y = 2

[ ]: print(x+y)
```

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

File Edit View Run Kernel Git Nbgrader Tabs Settings Help

Ex2.ipynb 6-311G-output.log

Filter files by name

■ / ... / Exercises / Ex2 /

Name	Last Modified
6-311G-output.log	9 months ago
6-31G-output.log	9 months ago
data_and_plots.ipynb	a month ago
Energy.dat	a month ago
eq_RHF-output.log	9 months ago
eq_UHF-output.log	9 months ago
Ex2.ipynb	2 minutes ago
IESM_Ex2_20220...	2 months ago
IESM_Ex2.ipynb	24 days ago
large_RHF-output.log	9 months ago
large_UHF-output.log	9 months ago
STO-3G-output.log	9 months ago
timer.dat	a year ago

```

6 *** tstart() called on noto.epfl.ch
7 *** at Wed Jan 26 17:15:38 2022
8
9 => Loading Basis Set ==
10
11 Name: 6-311G
12 Role: ORBITAL
13 Keyword: BASIS
14 atoms 1 entry H      line    21 file /opt/psi4conda/psi4conda-1.4rc3/share/psi4/basis/6-311g.gbs
15
16 -----
17
18 SCF
19       by Justin Turney, Rob Parrish, Andy Simonett
20           and Daniel G. A. Smith
21           UHF Reference
22           2 Threads, 1907 MiB Core
23
24
25 ==> Geometry <==
26
27 Molecular point group: d2h
28 Geometry (in Angstrom), charge = 0, multiplicity = 2:
29
30          Center        X          Y          Z          Mass
31          H        0.000000000000  0.000000000000  0.000000000000  1.007825032230
32
33
34 Running in d2h symmetry.
35
36 Rotational constants: A = ***** B = ***** C = ***** [cm^-1]
37 Rotational constants: A = ***** B = ***** C = ***** [MHz]
38 Nuclear repulsion =  0.000000000000
39
40 Charge = 0

```

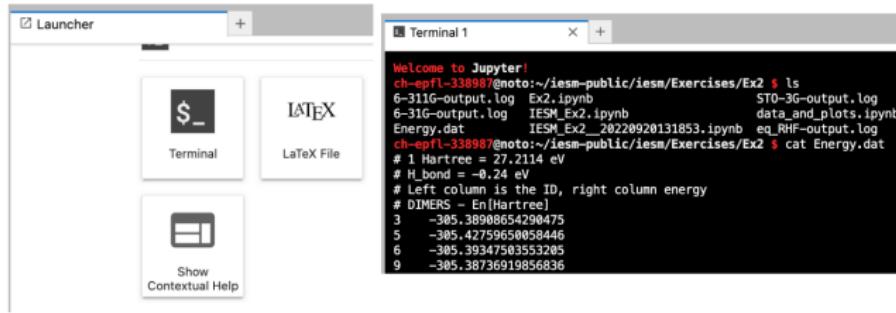
Linux & Terminal

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

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

iter	1:	-0.73775656591694	-7.37757e-01	2.26180e-02	DIIS
iter	2:	-0.74503745659583	-7.28089e-03	2.27444e-03	DIIS
iter	3:	-0.74511202947724	-7.45729e-05	5.15094e-06	DIIS
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

Understand what are basis functions

Get familiar with basis function notation

Basics of **Psi4**

Get familiar with molecular geometries

Chapter in script

Chapter 3 - Basis functions in quantum chemistry

Resources

Jensen, F. (2017). Introduction to computational chemistry.
John Wiley & Sons.

- Chapter 5 - Basis Sets

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 know 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 especially in the H₂O 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!