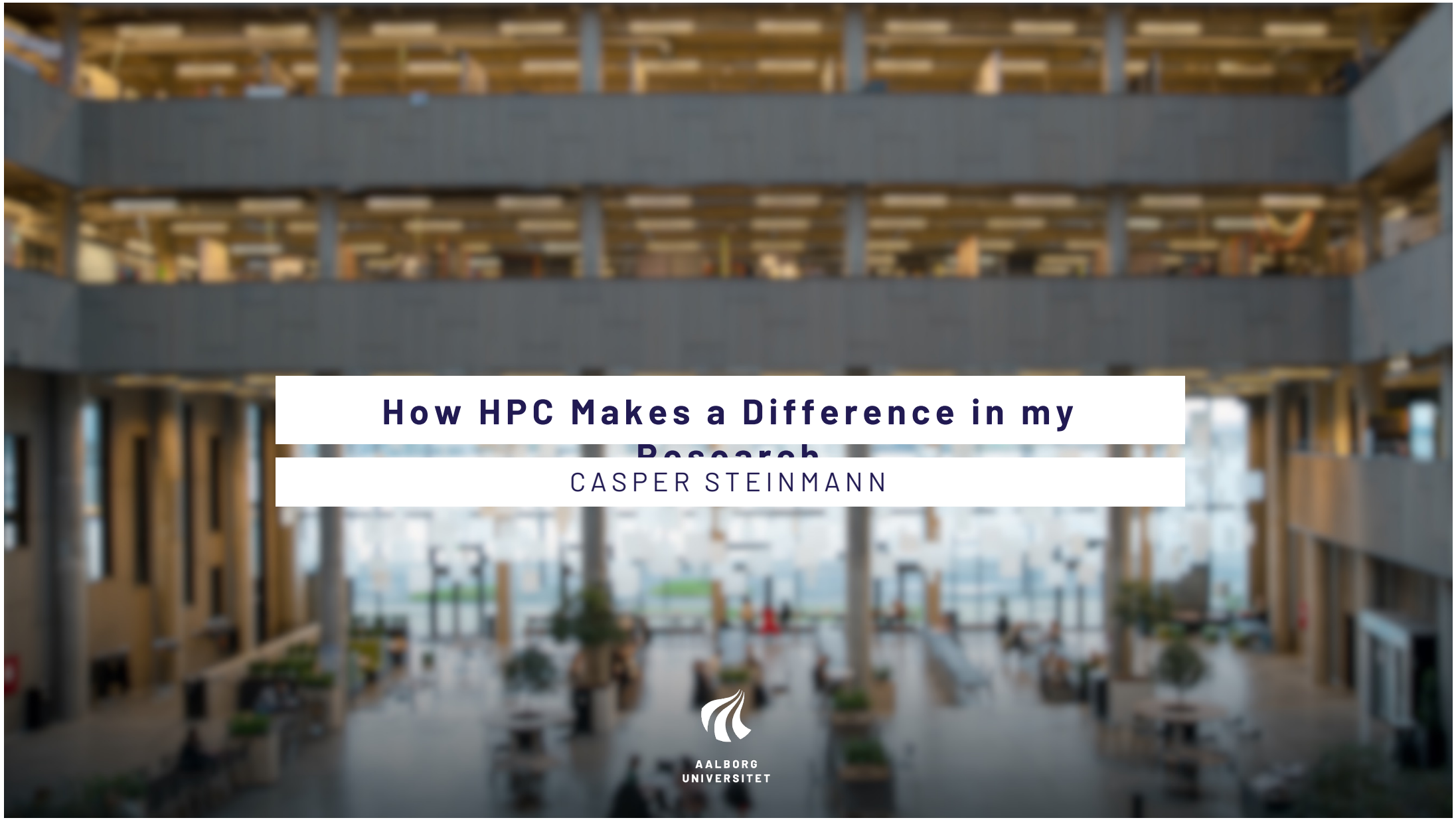


How HPC Makes a Difference in my Research

CASPER STEINMANN

AALBORG
UNIVERSITET

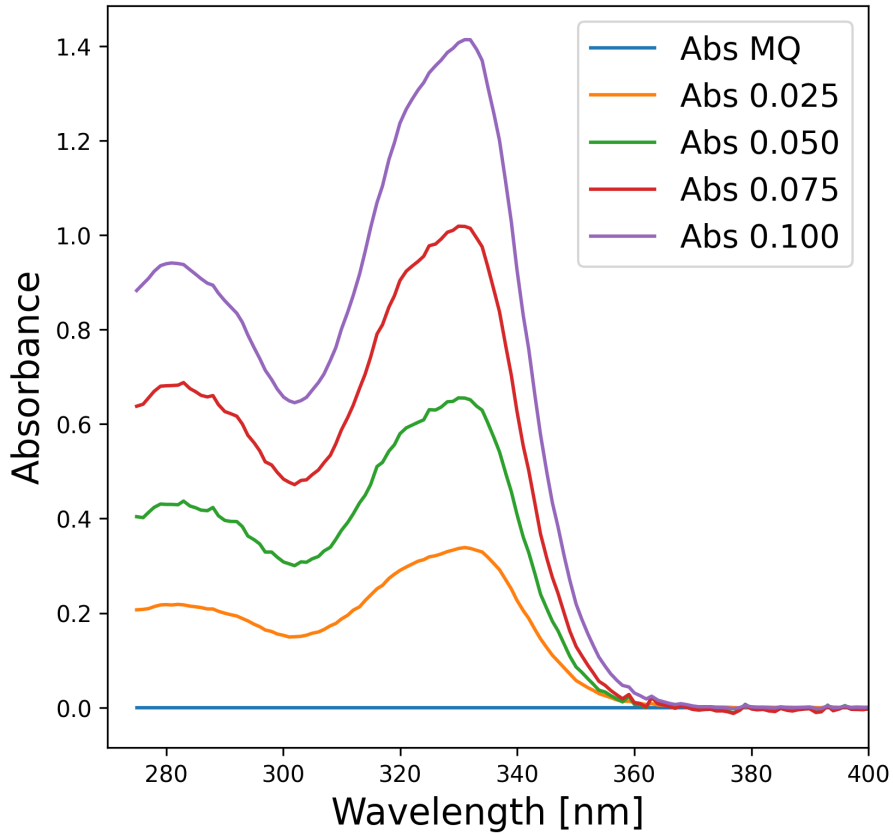
Casper Steinmann

- **Associate Professor in Computational Chemistry**
  - Applied Supramolecular Chemistry
- **Fundamental Research**
  Understanding the physics in chemistry with computational approaches
- **Method and Model Development**
  Accuracy, Speed, Insight, Idea Generation

A Simple Chemical Experiment

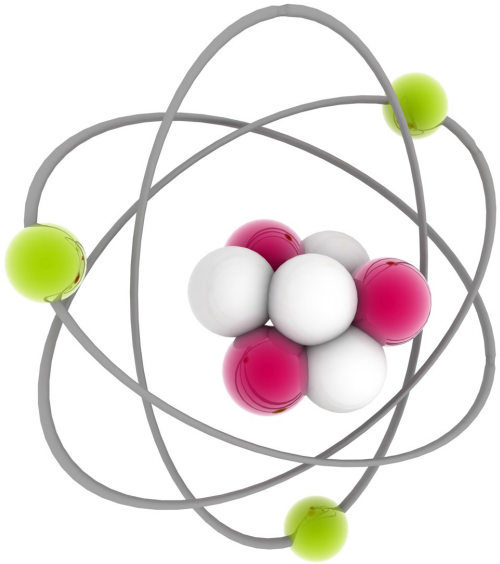

Please make sure You close the freezerdoor properly
Check that you hear the vacuum sound
3.319F

Molecular Fingerprints from Spectroscopy



How do you replicate experiments with computers?

$$\hat{H}\Psi = E\Psi$$



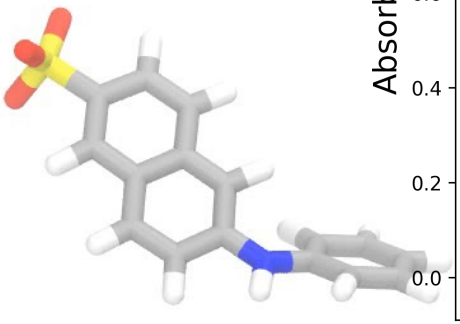
10^{23} molecules
10^{-14} seconds

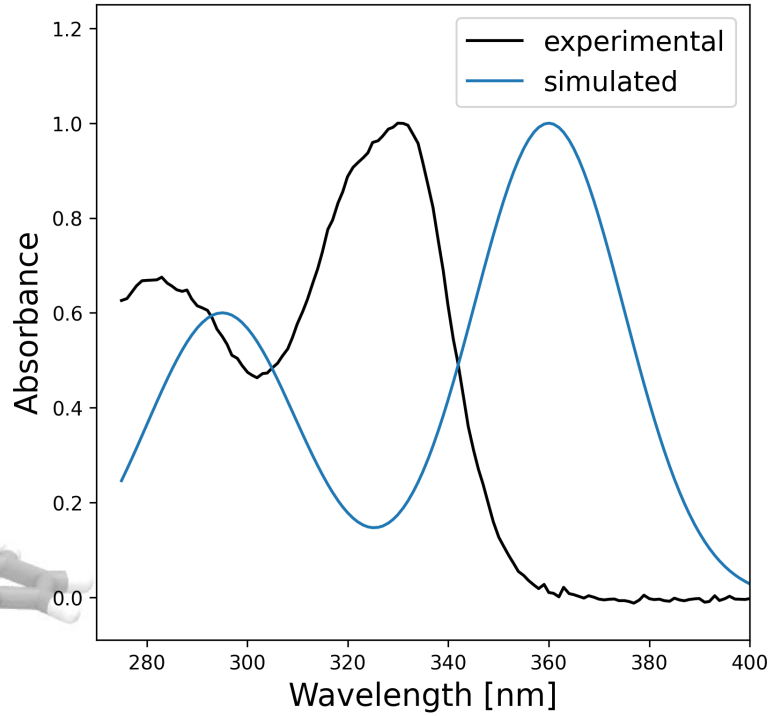
10^{3} molecules
10^{-9} seconds

$$\langle X \rangle =$$

Experimental

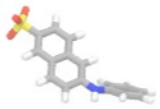
Simulated

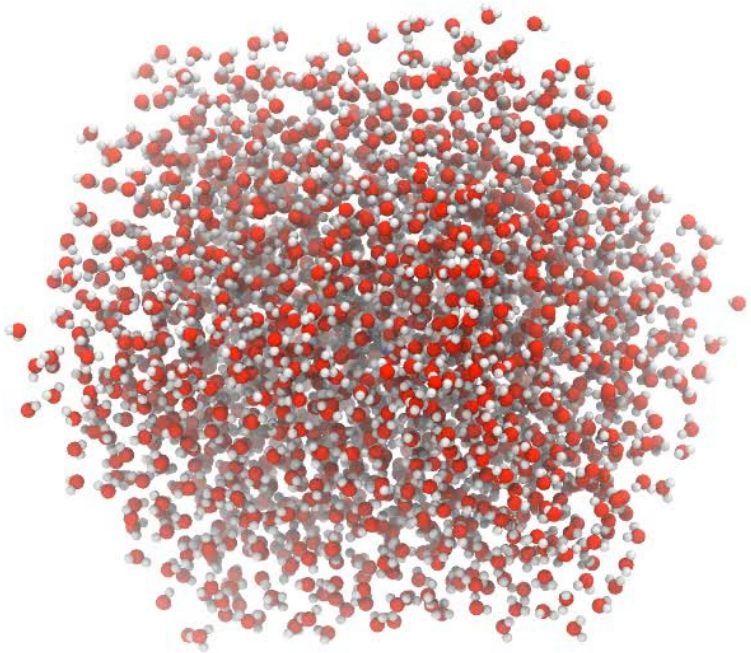


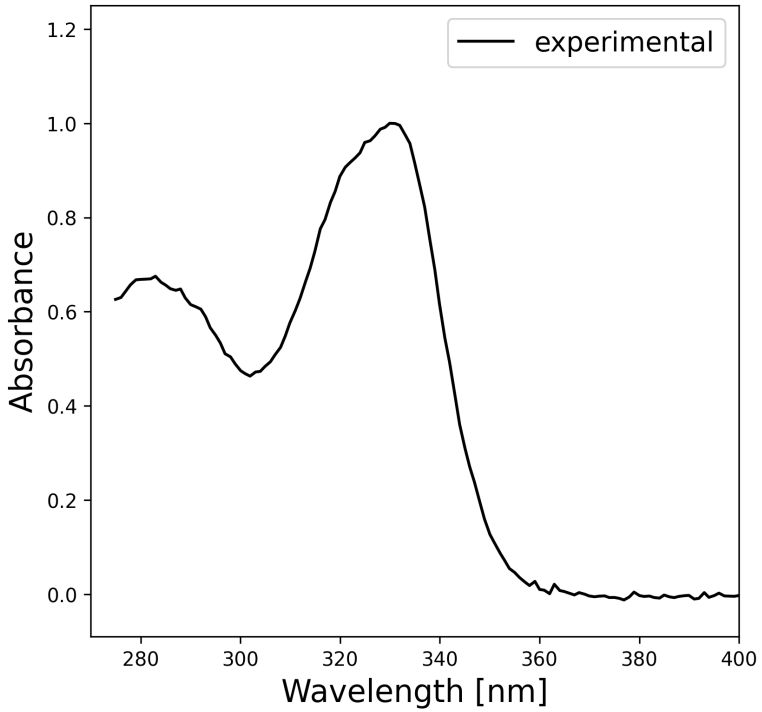


Simulation time:

5 minutes per snapshot
3 days on laptop
~ 5 minutes on HPC

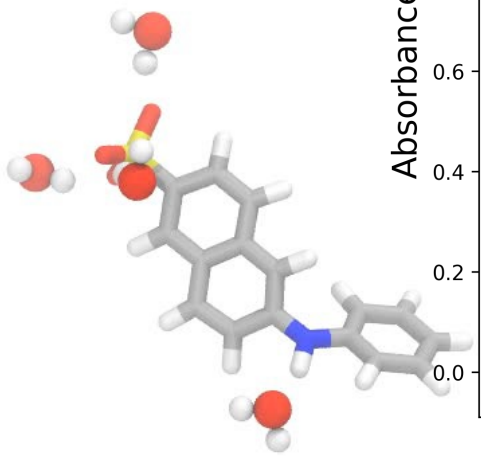


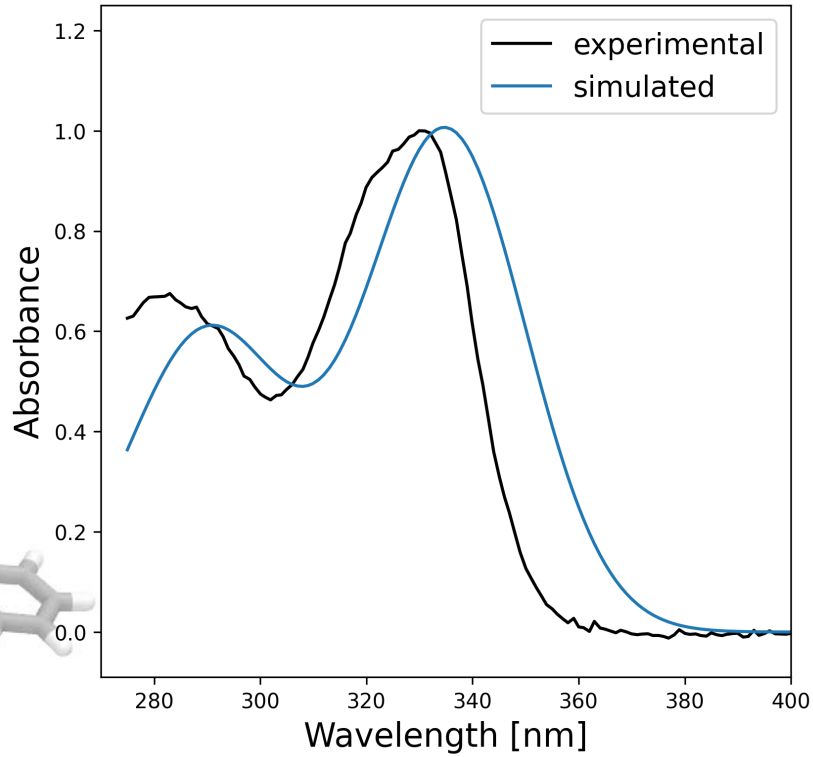




Simulation time:

- ∞ minutes per snapshot
- ∞ days on laptop
- ∞ on HPC



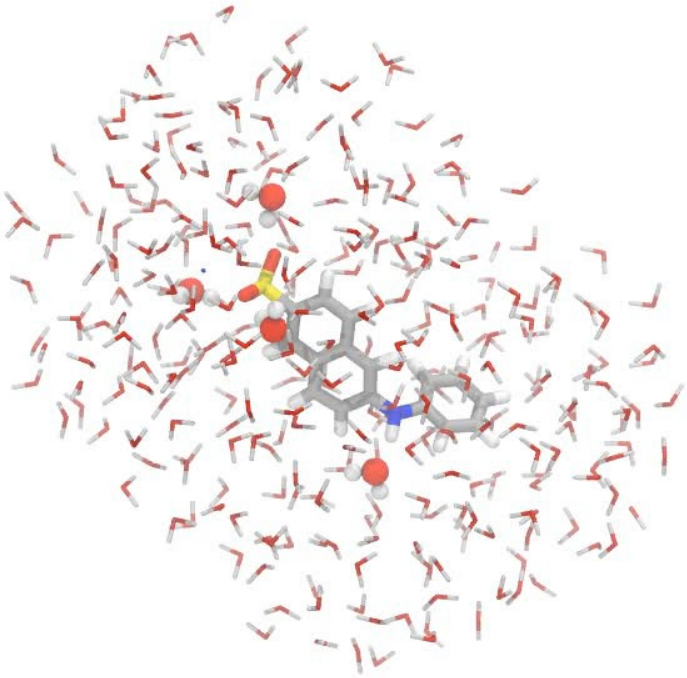


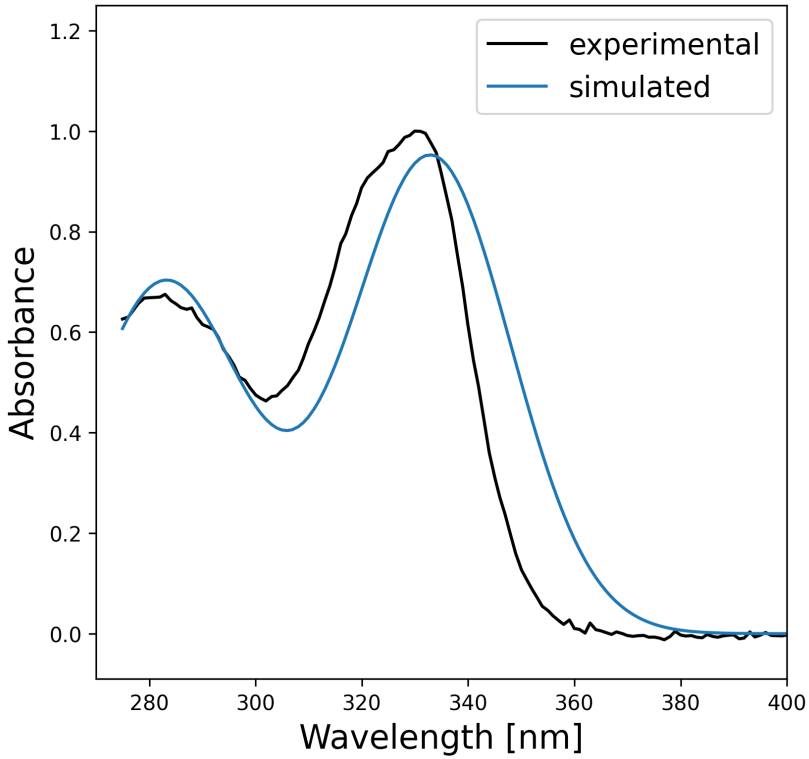
Simulation time:

120 minutes per snapshot

72 days on laptop

~1 day on HPC





Simulation time:

120 minutes per snapshot

72 days on laptop

~1 day on HPC

HPC and HPC with DeiC

- No High-Performance Computing – No Research.
- We need HPC due to the way that quantum mechanics scale.
  - Reproduction of experiments requires **lots** of computation. Prediction of experiments?
- DeiC application procedure is manageable.
- Shoutout to Niels Krogh Søndergaard for making lab video.

Thanks for Listening