Dive into computational physical chemistry

Lecture 1: Introduction

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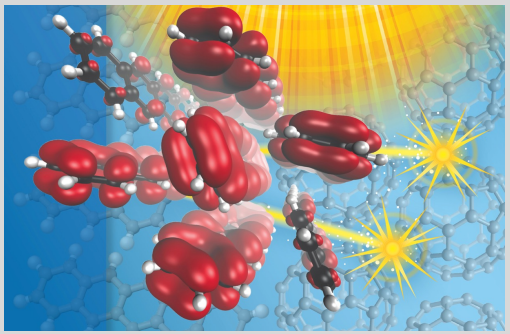
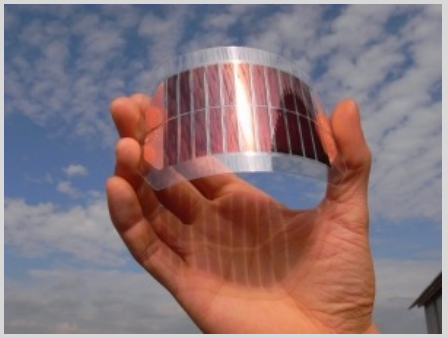
September 7, 2023

Two kinds of theoretical chemistry

Quantum Mechanics

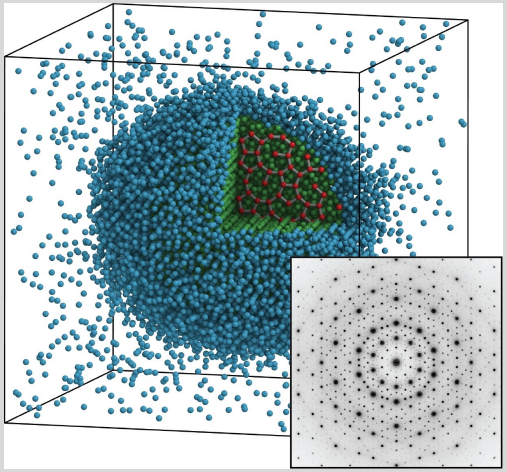
What is the behavior of the electrons?

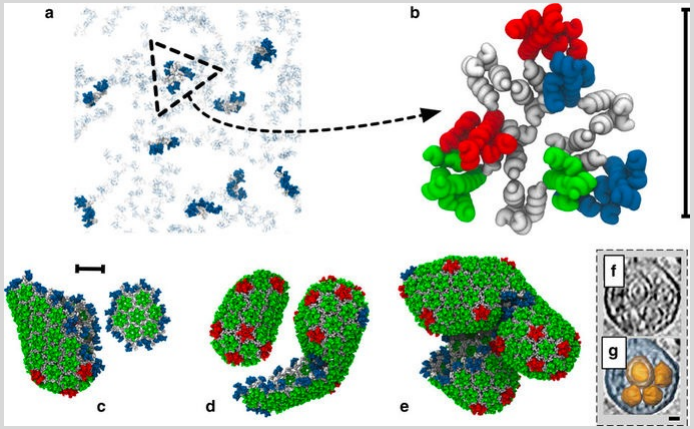




Statistical Mechanics

How do large collections of molecules behave?

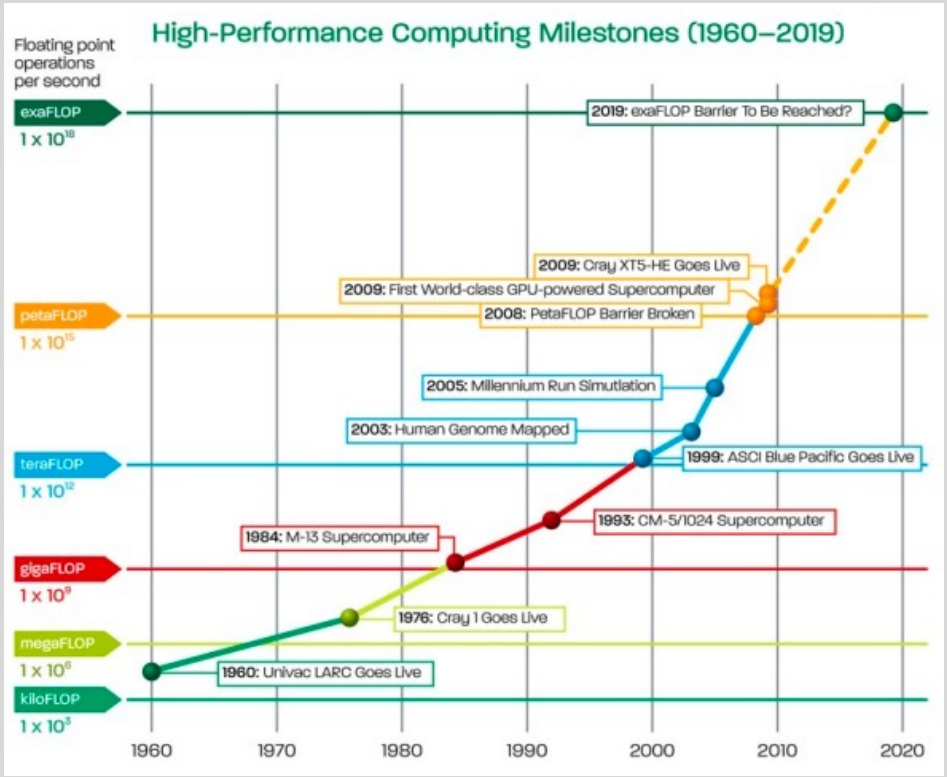


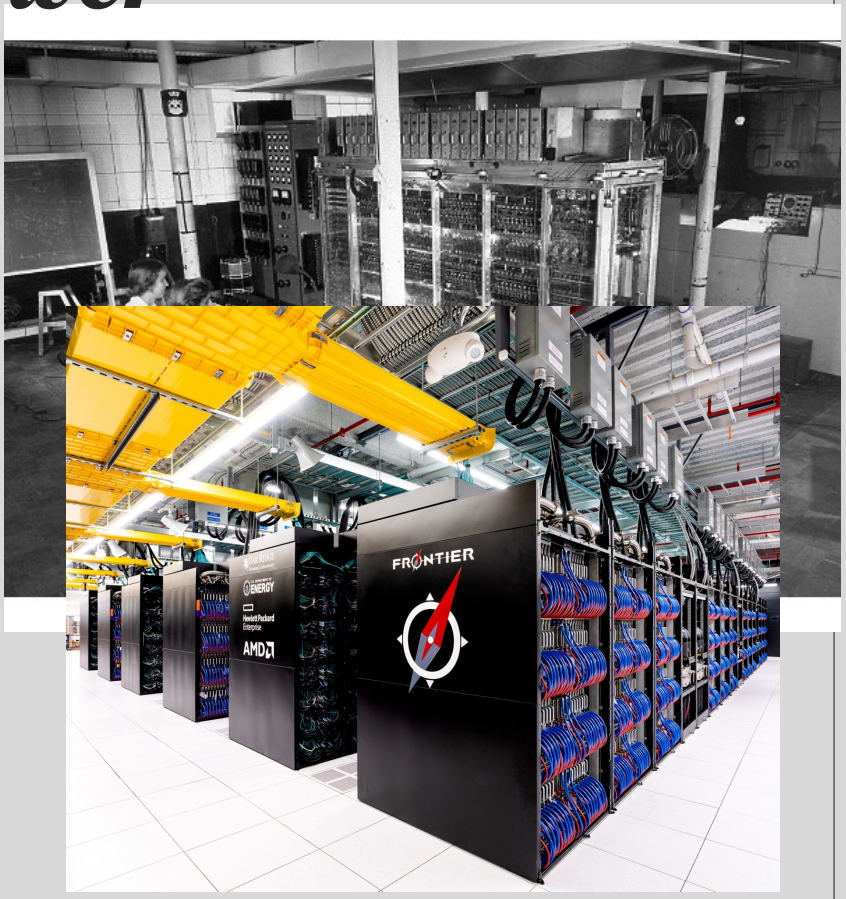


Need for computers

- Equations of quantum mechanics and of statistical mechanics are too complicated to solve by hand in most cases
- Used to make the most approximation that seemed reasonable, then sometimes use computers as calculators
- Computers first applied in chemistry during the Manhattan Project to predict nuclear properties

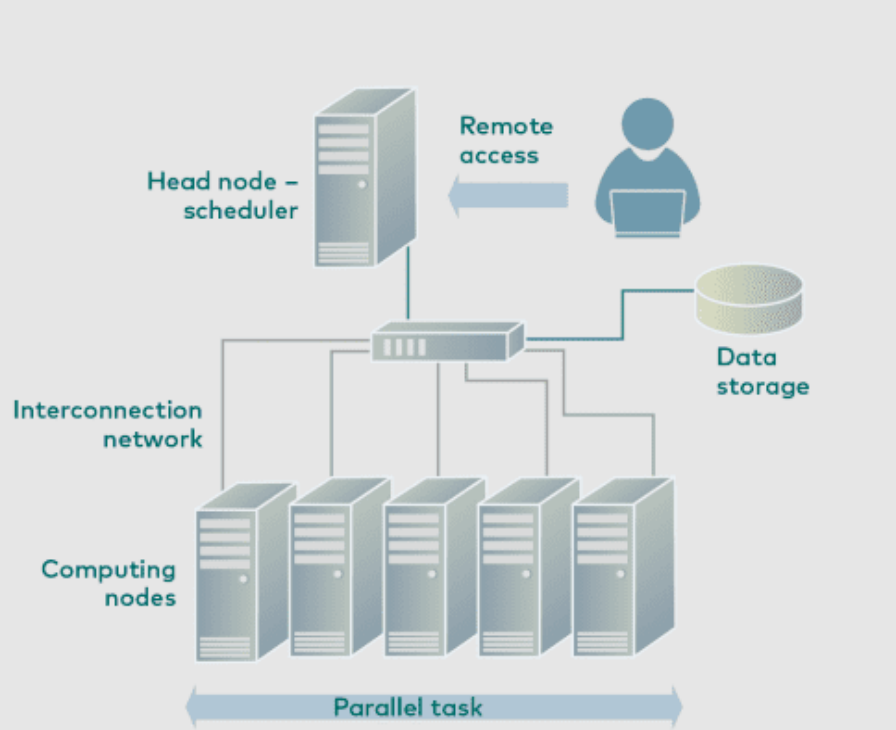
Advances in computing power





Frontier, ORNL, 1.01 exaflop. May 2022

High performance computing



NYU Greene (2022)

- The total number of nodes is 672
  - 6 login
  - 670 compute
    - 524 Standard memory (180 GB)
    - 40 Medium memory (360 GB)
    - 4 Large memory (3,014 GB)
    - 73 GPU RTX8000
    - 20 GPU V100
    - 9 GPU A100
  - 6 administrative
- The total number of CPU cores is 31,584
- The total number of GPU cards is 368 (292 RTX8000 with 48GB; 76 V100 with 32GB)
- The total memory is 163 TB

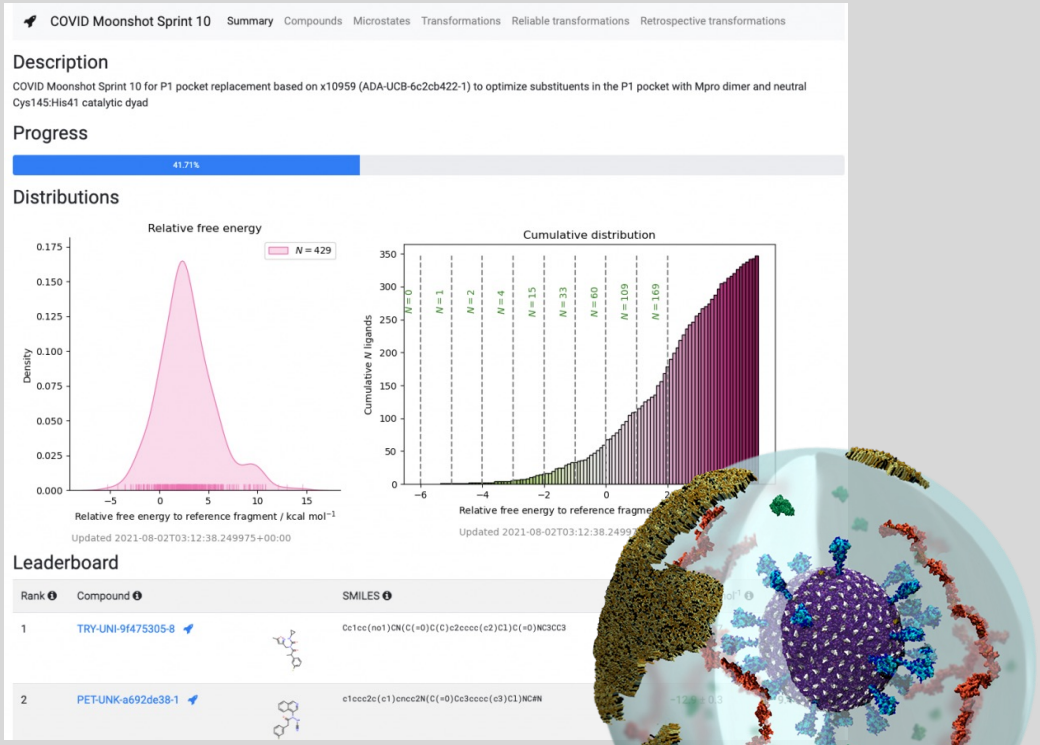
https://sites.google.com/nyu.edu/nyu-hpc/home

Different types of parallel computing

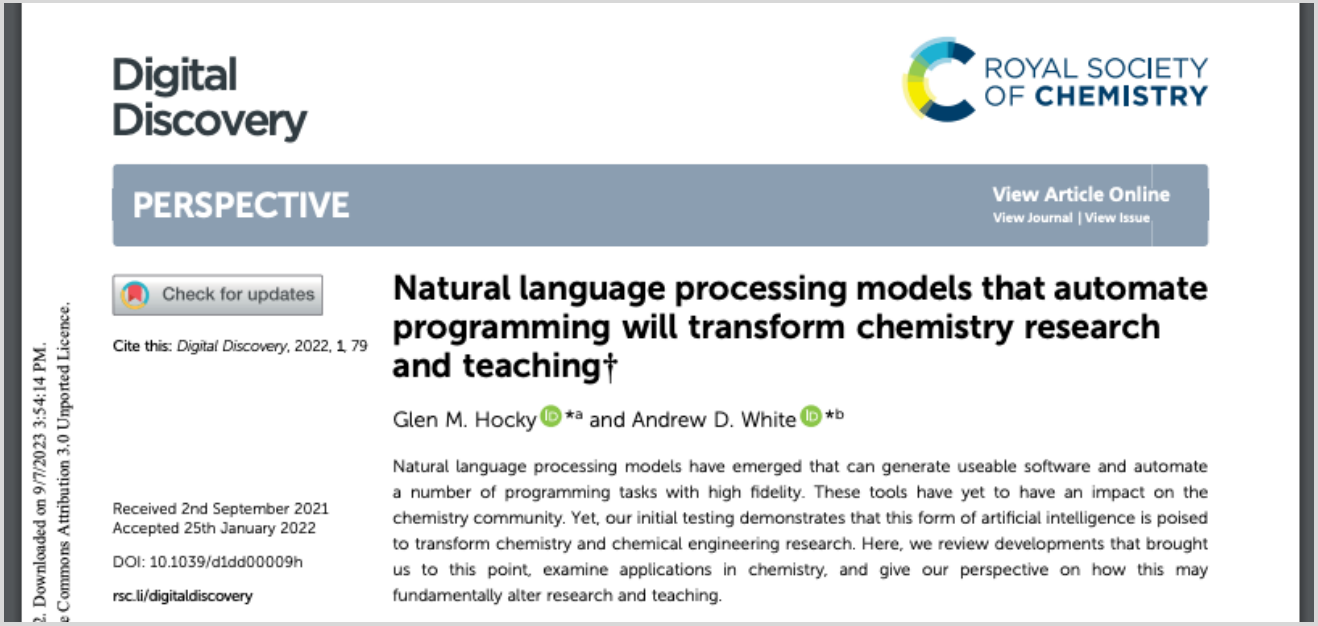
- Trivial/many task
- Tightly coupled, requires communication (e.g. MPI)
- Shared memory – OpenMP, GPU

Typically we will do hybrid, many tasks each of which are accelerated through parallel process (discussed in a later lab)

Example uses of computational chemistry



Next frontier, LLMs in chemistry



Digital Discovery

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Natural language processing models that automate programming will transform chemistry research and teaching†

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Natural language processing models have emerged that can generate useable software and automate a number of programming tasks with high fidelity. These tools have yet to have an impact on the chemistry community. Yet, our initial testing demonstrates that this form of artificial intelligence is poised to transform chemistry and chemical engineering research. Here, we review developments that brought us to this point, examine applications in chemistry, and give our perspective on how this may fundamentally alter research and teaching.

Class logistics

Discussion of syllabus:

https://hockygroup.hosting.nyu.edu/teaching/comp/syllabus/ComputationalLab_GA2671_Syllabus_2023_draft.pdf

Discussion of slack:

https://nyu-chem-ga-2671-2023.slack.com/

Today:

- The BASH shell and linux file system
  - Directory trees, relative directories, links [make your own directory in class /scratch/work space]
  - Moving and creating commands, eg cd, ls, pwd, mkdir
  - Man pages
  - Modules
- Secure shell (ssh) introduction, log in to greene on the command line
- https://ood.hpc.nyu.edu – running a jupyter notebook or interactive
- Text editing on the command line (VIM, emacs, nano)
- Creating and discussing ssh keys
- (Adding ssh key to github)
- Taking a quick look at github copilot / chatGPT / BingChat
- What is git/github? A quick introduction to version control. A tour around an example project
- Example chemistry software - VMD