# Dive into computational physical chemistry
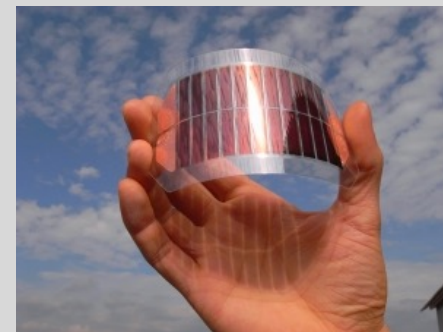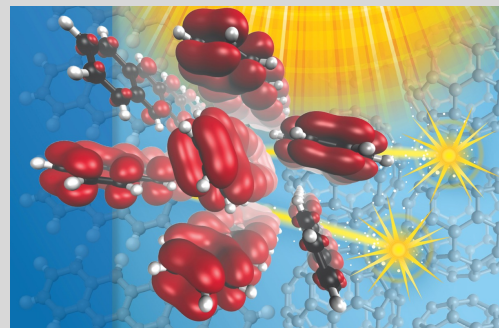
# Lecture 1: Introduction

Glen Hocky

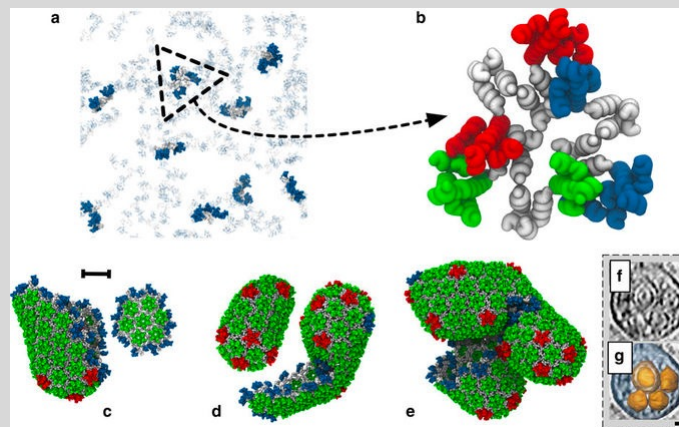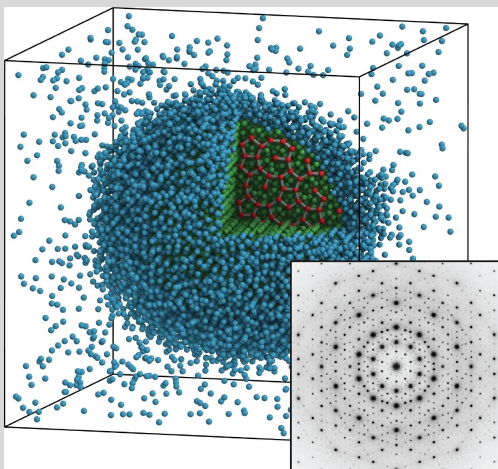September 6, 2022

# *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

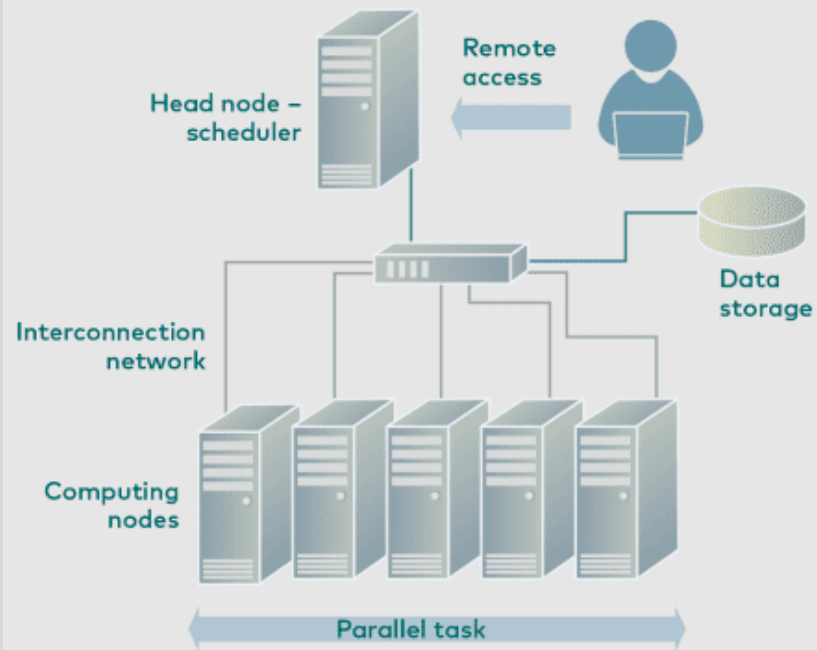- Computers first applied in chemistry during the Manhattan Project to predict nuclear properties
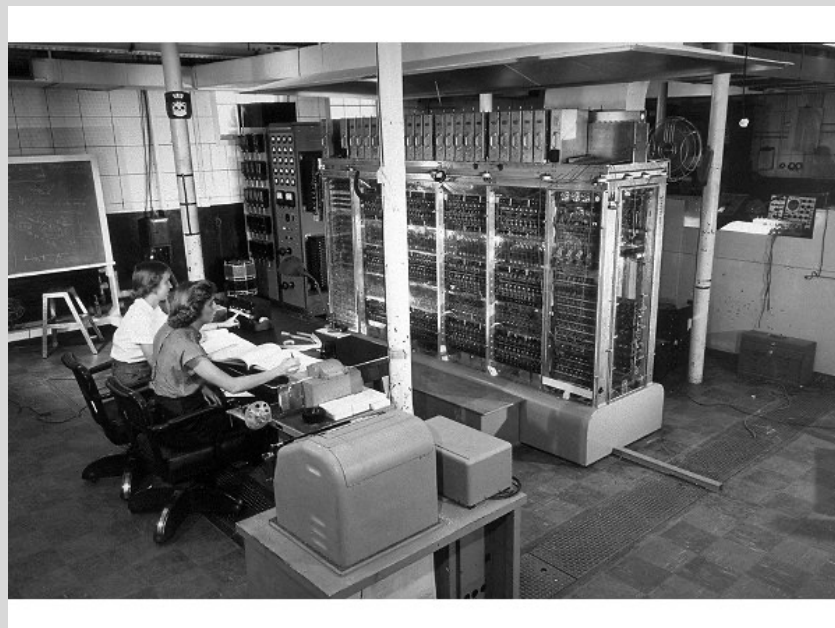
# Advances in computing power
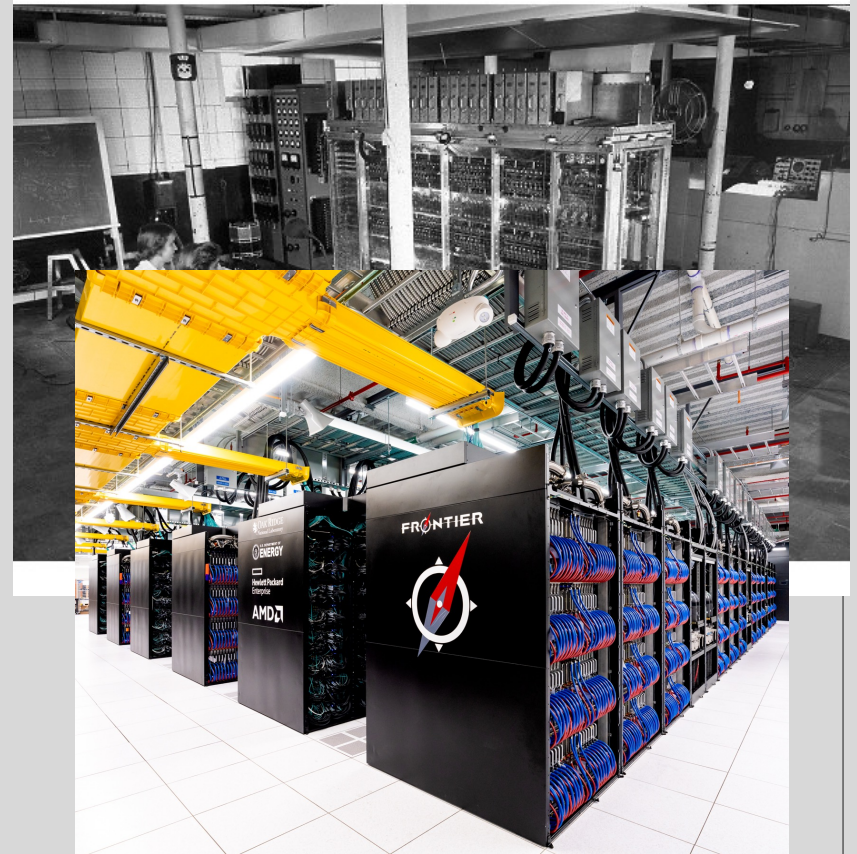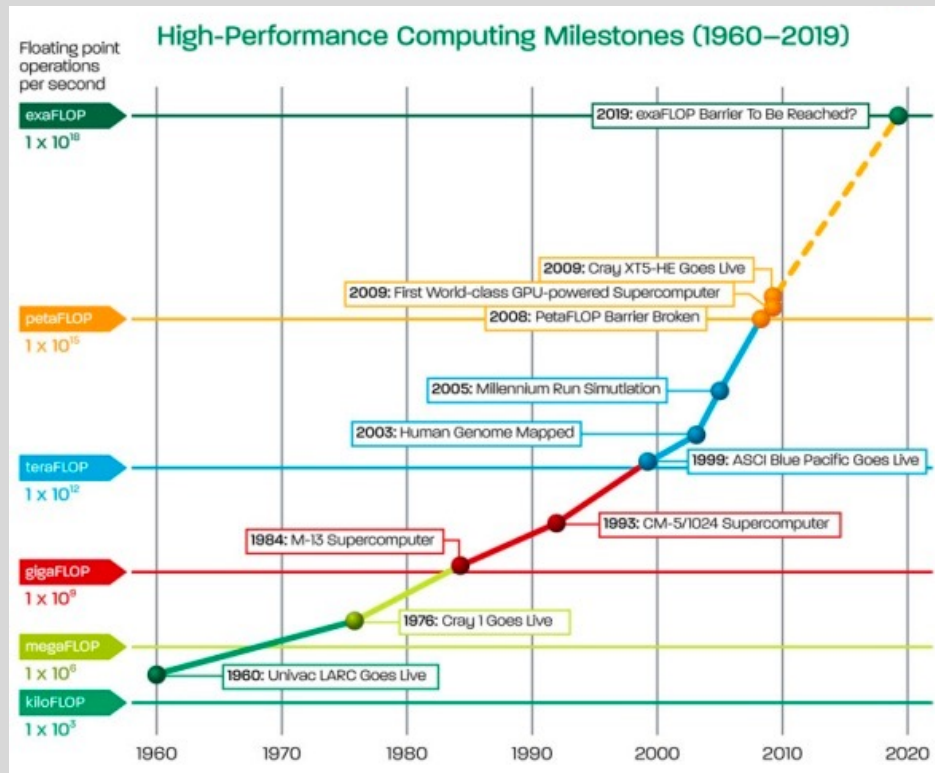


Frontier, ORNL, 1.01 exaflop. May 2022

# 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

# *Class logistics*

◦ See syllabus

https://hockygroup.hosting.nyu.edu/teaching/comp/syllabus/ComputationalLab_GA2671_Syllabus_2022_draft.pdf

# *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 (also try OOD)

◦ 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

◦ What is git/github? A quick introduction to version control. A tour around an example project

◦ Example chemistry software - VMD