Instructions for Major exam

- Major exam: 12th April 2022, 2:15 pm-4:15 pm, LH108 and LH521.
- One hour exam on MOODLE in OFFLINE mode.
- Syllabus: Lectures taught after the MINOR exam.
- Please make sure that your laptop battery is working fine and can hold charge upto 1.5 hrs atleast.
- Please ensure that your laptop is able to connect to the IITD network without any hardware issues.
- No excuse of laptop getting discharged or any technical faults will be considered. In such a case, no request for Viva or re-major will be considered. It is your responsibility to ensure that your exam can go smoothly.
- All of you must attempt the exam. No re-major /viva requests will be entertained at any cost.

Lecture 35

Molecular dynamics simulations

Textbooks:

- Computational Materials Science: J. Gunn Lee
- Molecular Modelling Principles and Applications: Andrew Leach (Chapter 4)
- Understanding Molecular Simulations: D. Frenkel and B. Smit (Chapter 4)

Prof. Divya Nayar
Department of Materials Science and Engineering
divyanayar@mse.iitd.ac.in

Recap…

- Computational materials science: Introduction
- Modeling in simulations: potential energy surface and multi-scale modeling
- Developing a model

Computational experiment: *Recipe*

Turning complex ideas into solvable equations

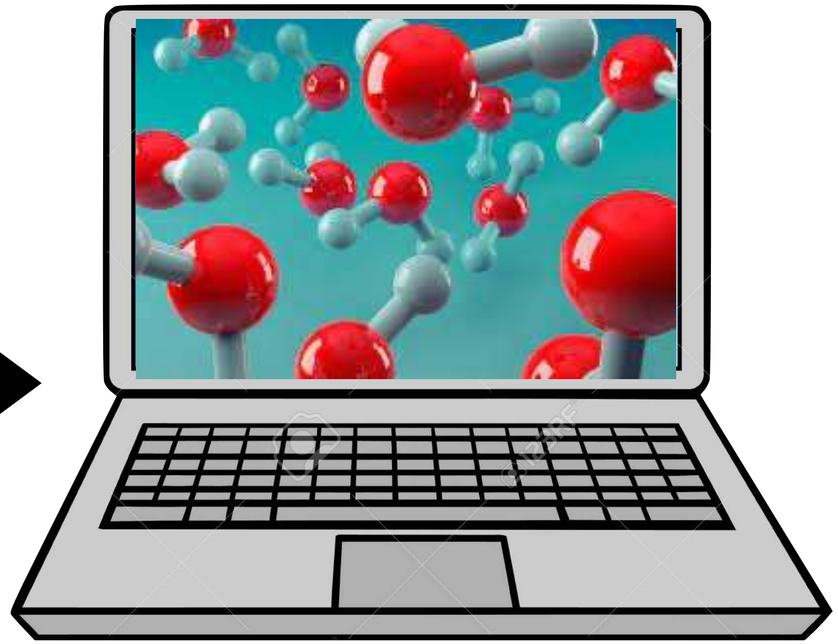
Define a problem

✓

Build a model

✓

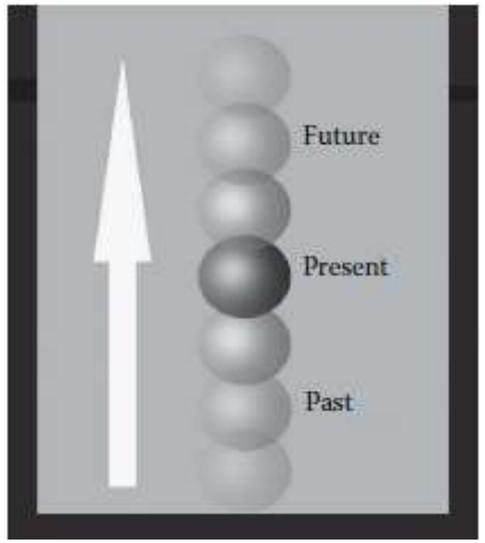
?



- Theory: set of rules to follow
- Simulation: algorithm to solve the problem
- Computer: ???

Google images

Classical Systems



Thermal de Broglie wavelength

$$\Lambda = \frac{h}{2\pi m k_B T}$$

h = Planck's constant
T= temperature
m = mass of particle
k_B= Boltzmann's constant

For a system to be classical, the wavelength should be much lesser than the inter-particle spacing $\Lambda << d$

Hamiltonian for electronic systems

$$\hat{H} = \sum_{i=1}^{N} \left(\frac{-h}{2m_i} \nabla_i^2 + \hat{V}_i \right)$$

Kinetic energy operator — Potential energy operator

Hamiltonian for classical systems

$$H = \sum_{i}^{N} \frac{p_i^2}{2m_i} + U(r_1, \cdots, r_N)$$

Kinetic energy — Potential energy

6N-dimensional hypersurface (phase space)

Computational Materials Science: An Introduction; J. G. Lee

Opening lines of "States of Matter", D.L. Goodstein

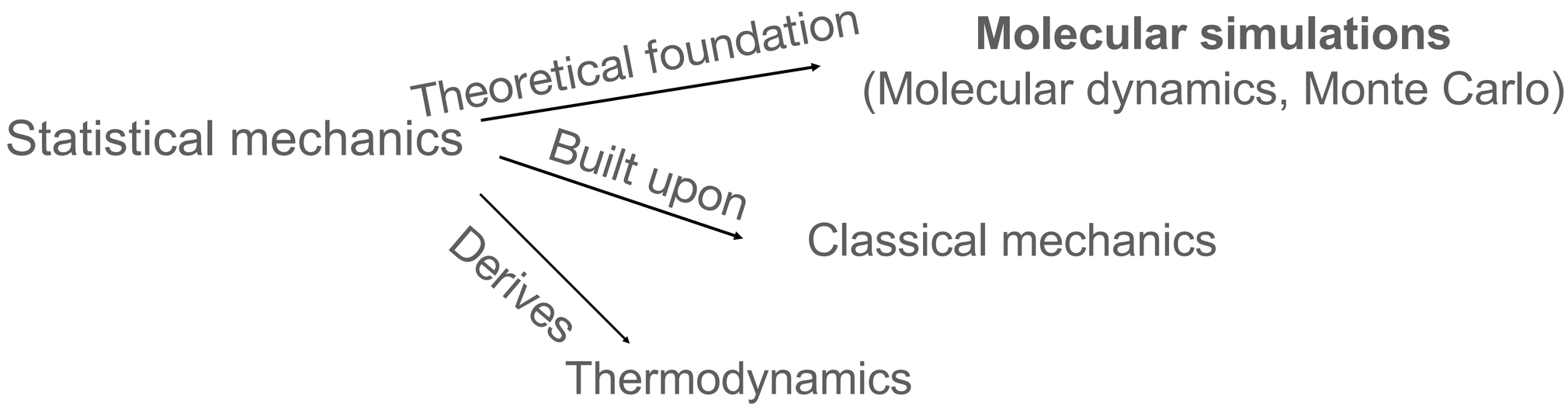
STATISTICAL MECHANICS

1.1 INTRODUCTION: THERMODYNAMICS AND STATISTICAL MECHANICS OF THE PERFECT GAS

Ludwig Boltzmann, who spent much of his life studying statistical mechanics, died in 1906, by his own hand. Paul Ehrenfest, carrying on the work, died similarly in 1933. Now it is our turn to study statistical mechanics.

Perhaps it will be wise to approach the subject cautiously. We will begin by considering the simplest meaningful example, the perfect gas, in order to get the central concepts sorted out. In Chap. 2 we will return to complete

Statistical Mechanics (The Theory)



Some definitions

- **Microstate**: A state or configuration of the system in which the constituent elements i.e. 3N position and 3N momentum coordinates are specified.

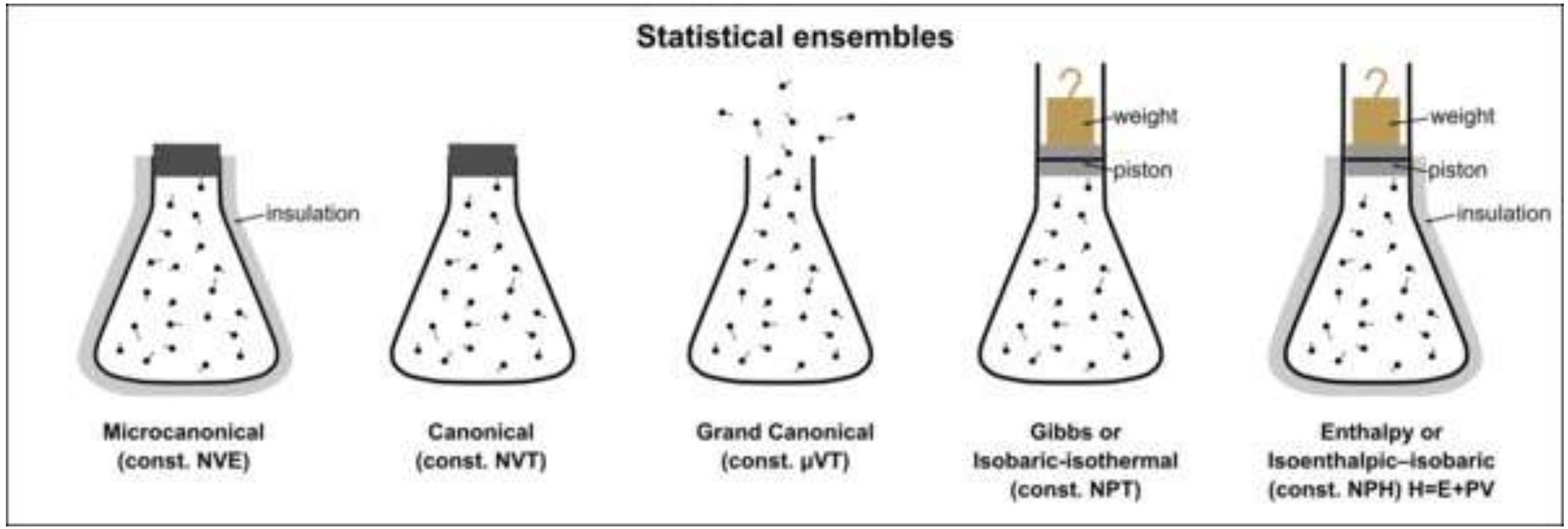
$$\{\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N; \vec{p}_1, \vec{p}_2 \ldots \vec{p}_N\}$$

- **Ensemble**: A collection of microstates satisfying some common set of macroscopic constraints.

- **Partition function**: Sum over all possible microstates weighted by probability of occurrence of microstates in the ensemble.

Ensembles

Ensembles

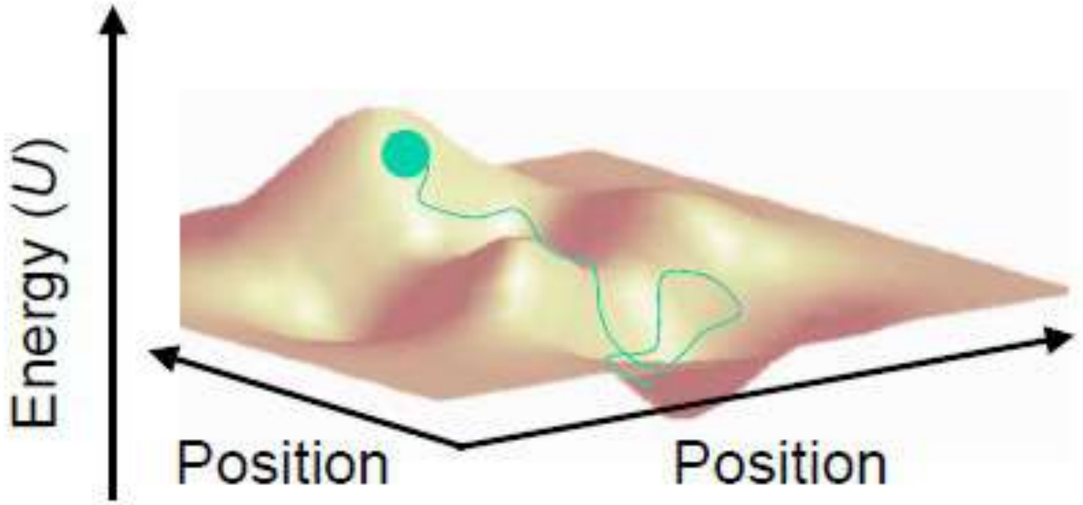


Isolated Closed Open Closed Closed

N= no. of particles
V= volume of the system
E= total energy of the system
T= temperature
P= pressure

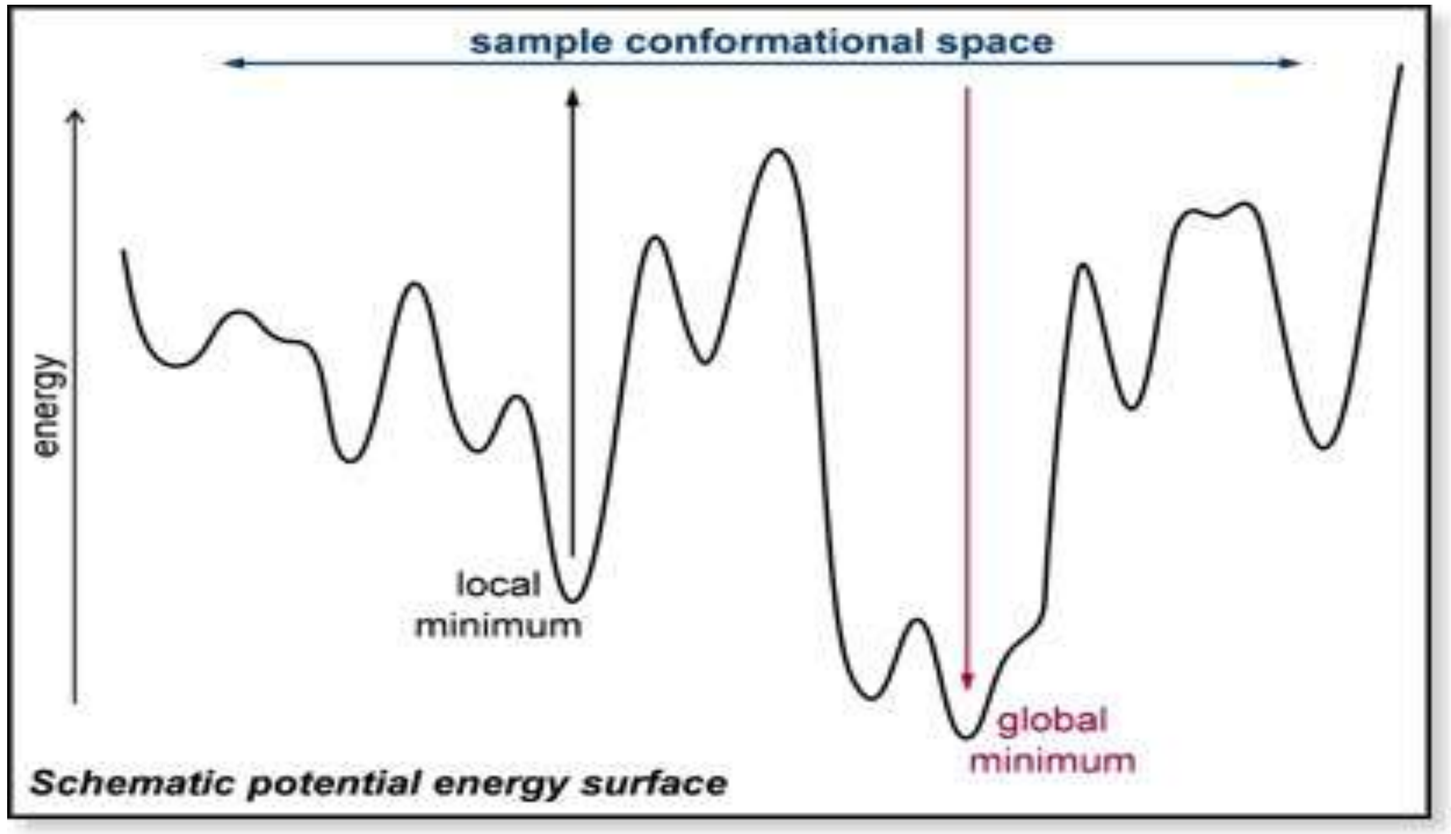
Basic Idea of molecular dynamics simulation

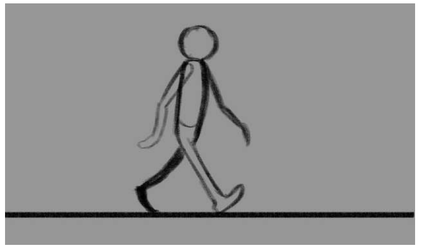
- Mimic the behaviour of atoms in real systems.
- The potential energy function allows to calculate the force experienced by each atom due to the others.
- Newton’s law governs the motion of atoms.
-The average behaviour of the system can be observed by sampling all possible points on this landscape.



Potential Energy Surface or Potential Energy Landscape

- Each point in the energy landscape corresponds to a “microstate” or configuration of the system
- Target is to sample as many microstates or configurations as possible to obtain an average behaviour or property of the system.

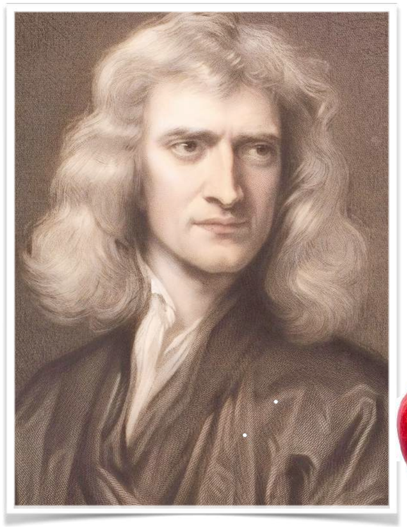




https://labs.chem.ucsb.edu/bowers/michael/theory_analysis/mm/sampling.shtml

Molecular dynamics simulations

Newton's second law of motion

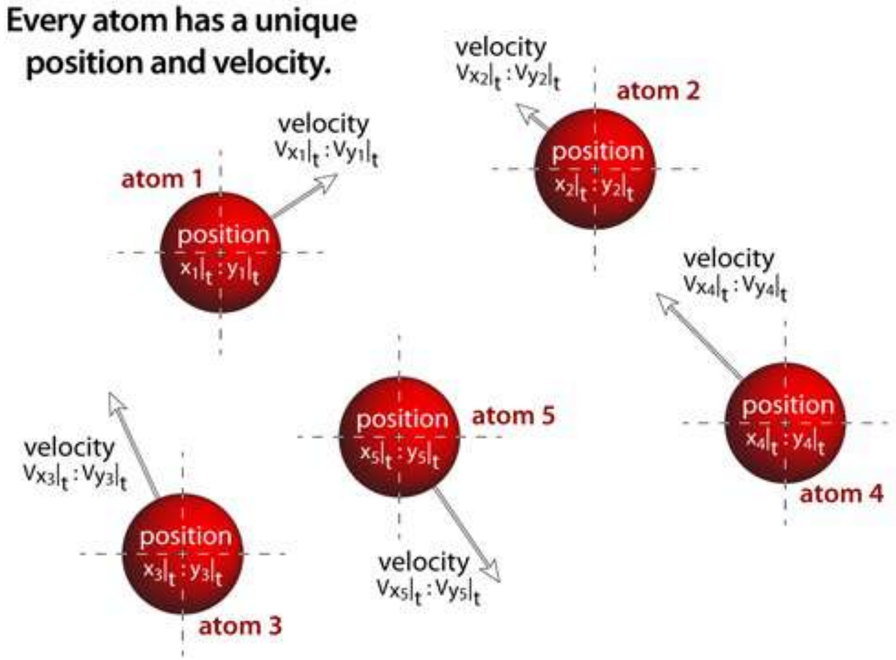


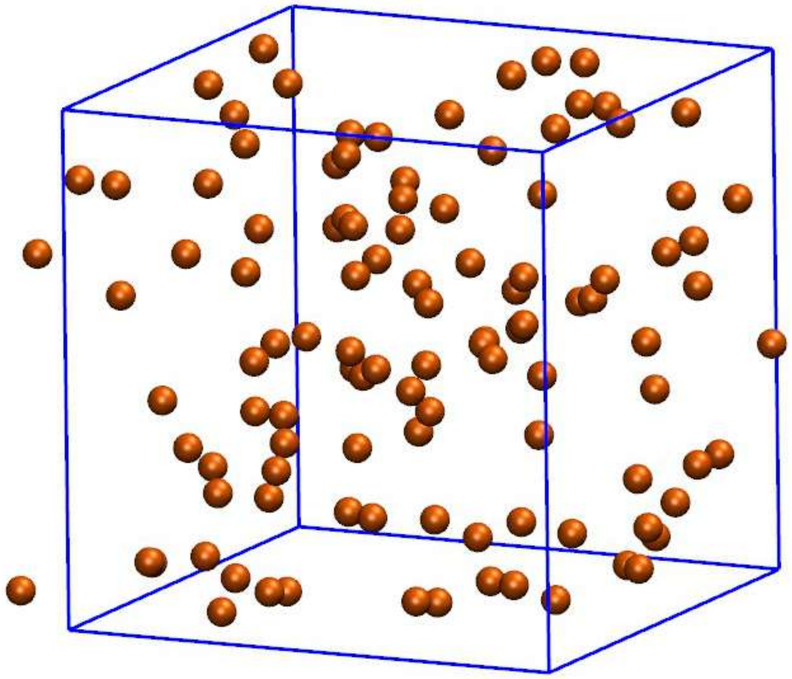
$$\vec{F} = m\vec{a}$$

$$\overrightarrow{F_i} = m_i \frac{d^2\overrightarrow{r_{ij}}}{dt^2} = -\nabla U(\overrightarrow{r_{ij}})$$

6N-coupled second order differential equations

$$U(\mathbf{r}) = \frac{1}{2}\sum_i \sum_{j \neq i} u_{pair}(r_{ij})$$

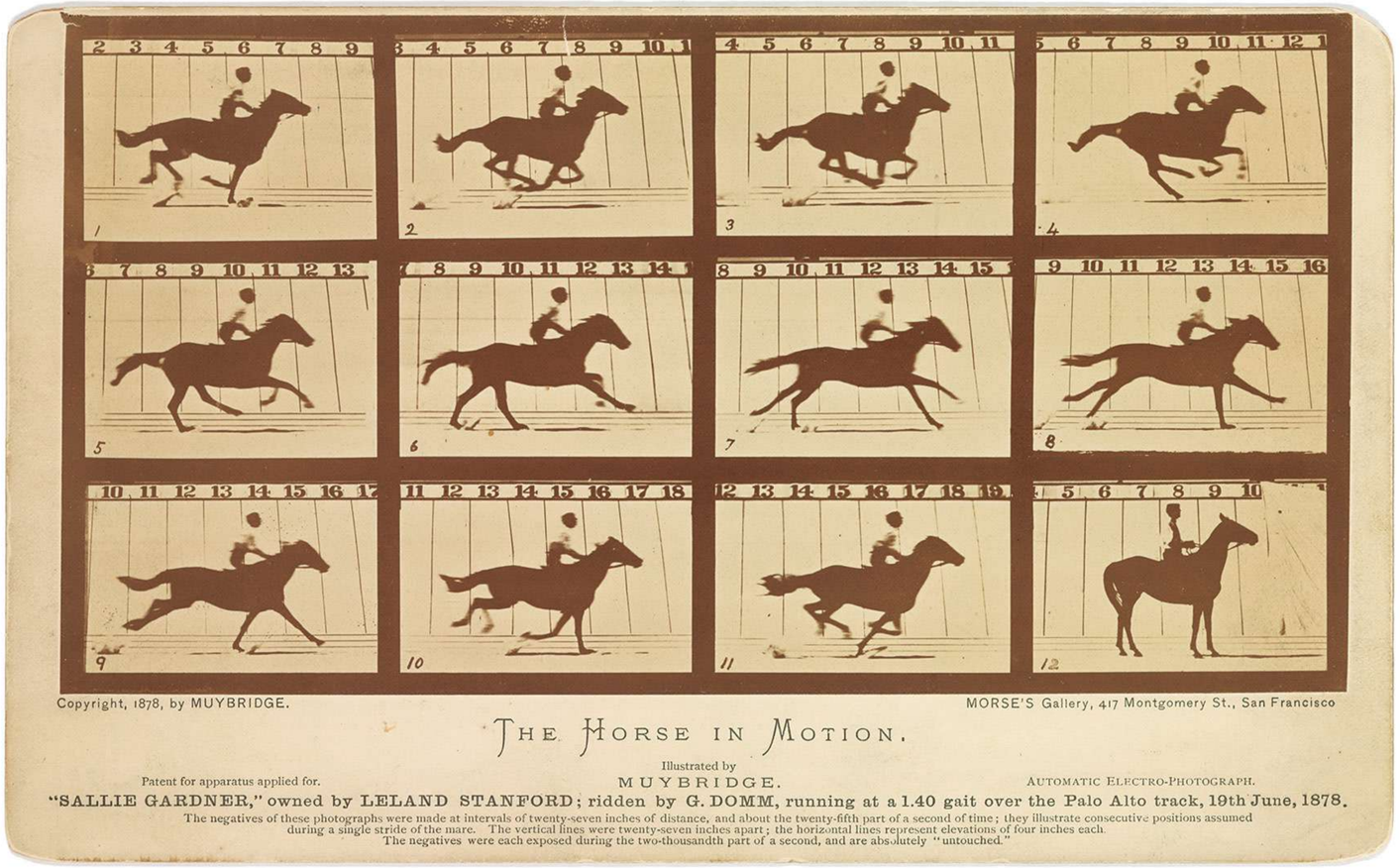




Molecular *dynamics* simulations

In MD, the natural time evolution of a system is computed and the quantity of interest is averaged over a sufficiently long time.

t=0

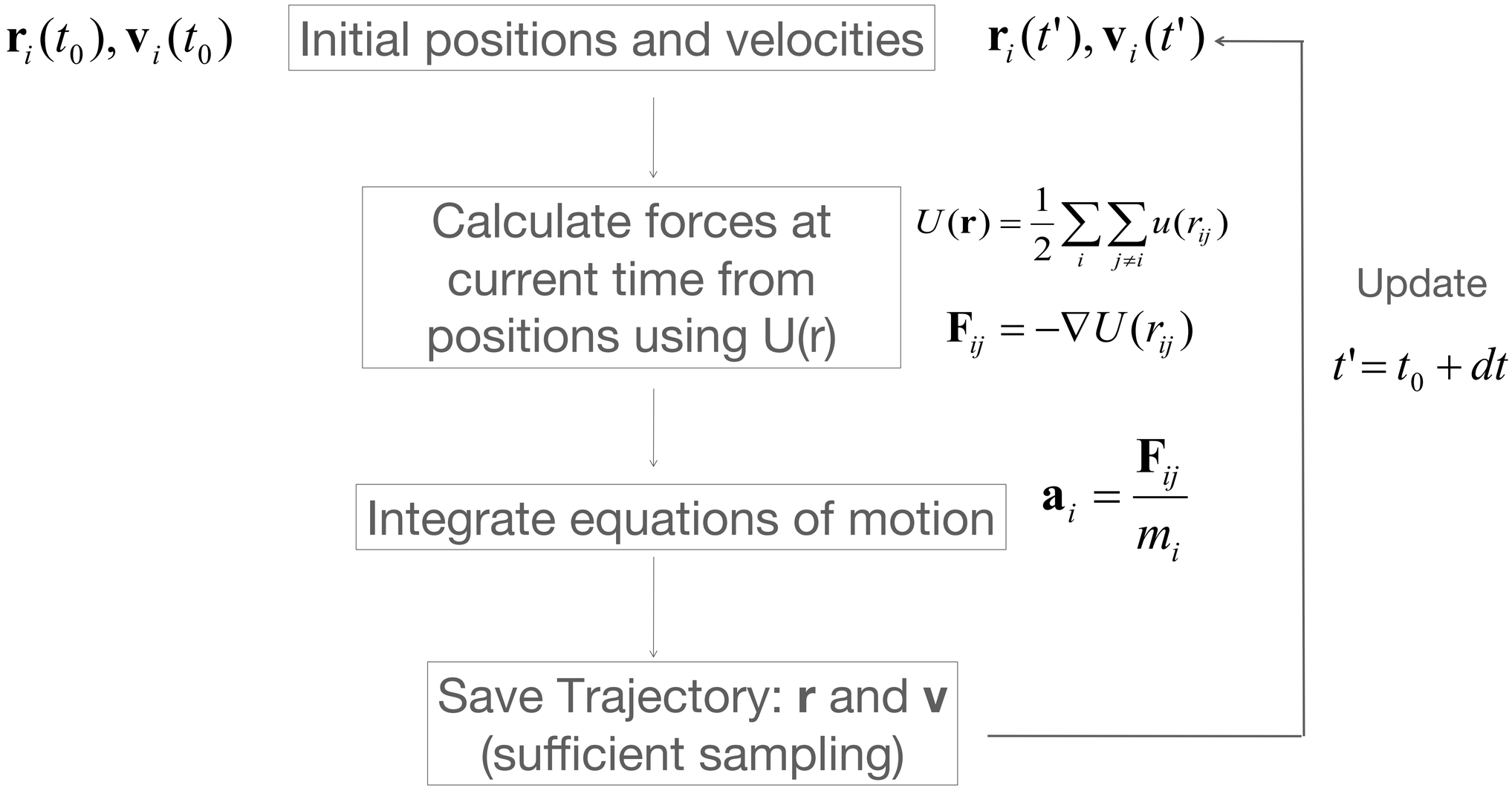


t=10 mins

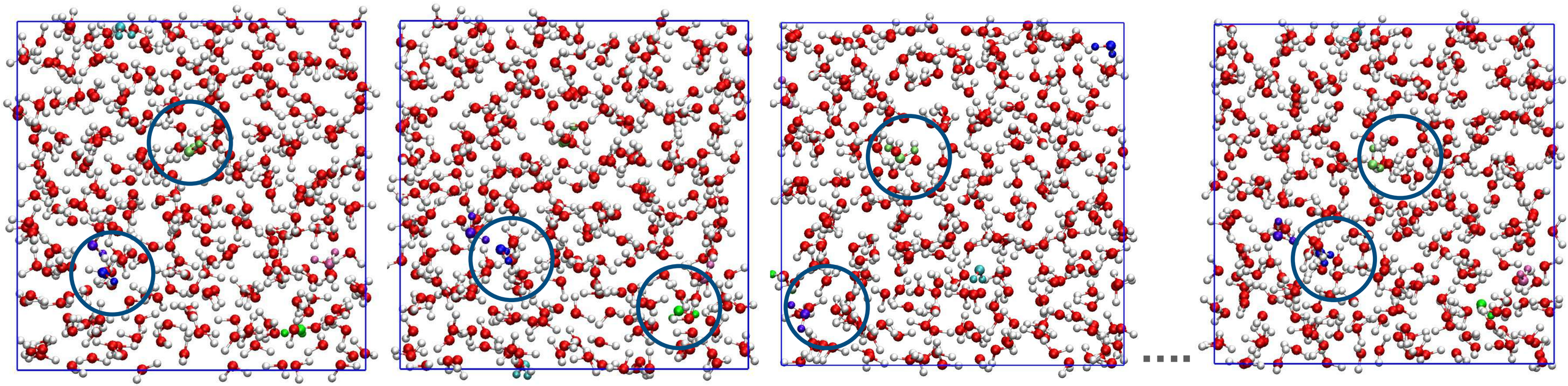
Google images

A nice book to read-Molecular Dynamics Simulations: Elementary Methods by J. M. Haile

Structure of MD algorithm



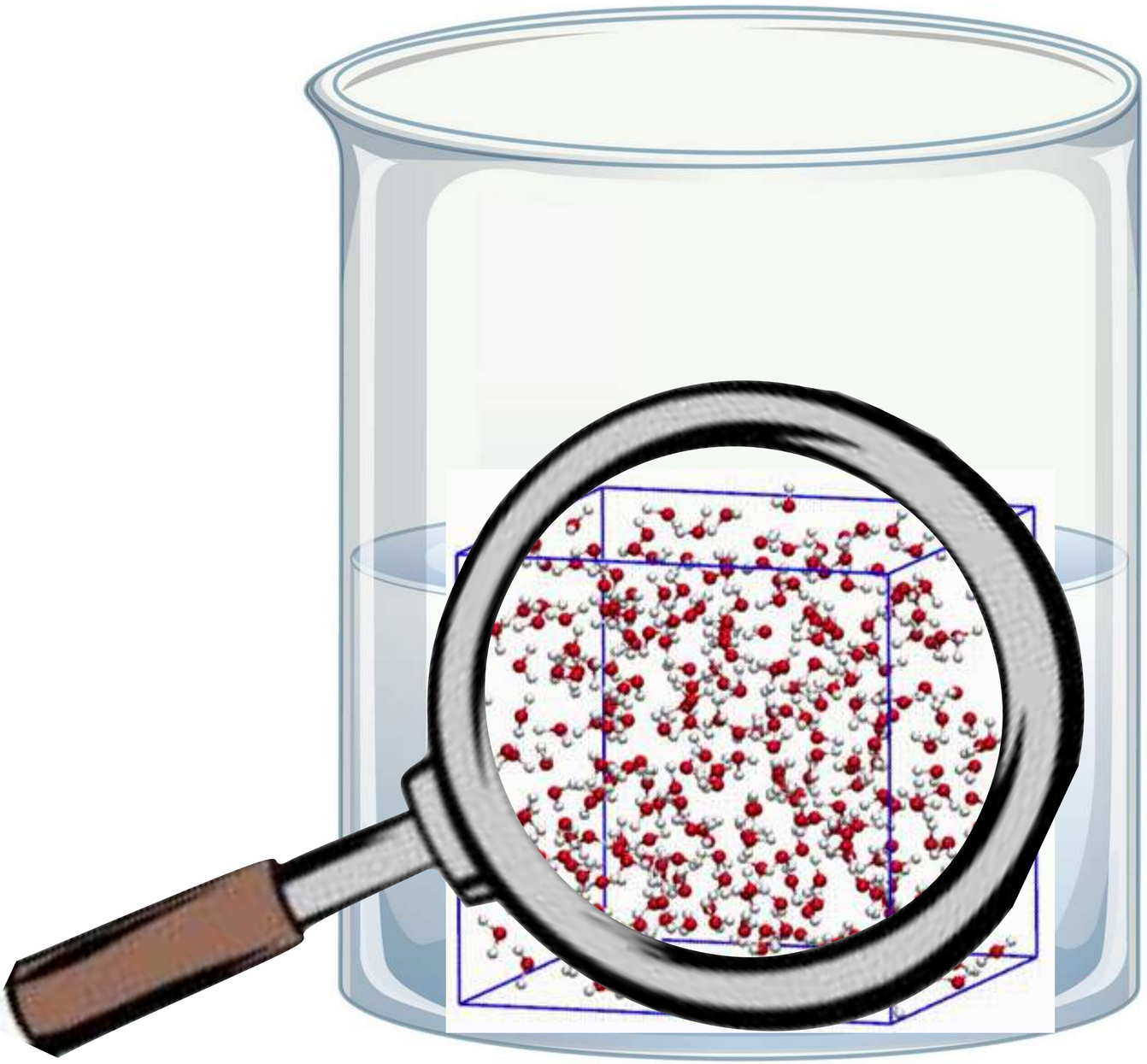
Observing the behaviour of water over time



t=0 .... t=T (ns)

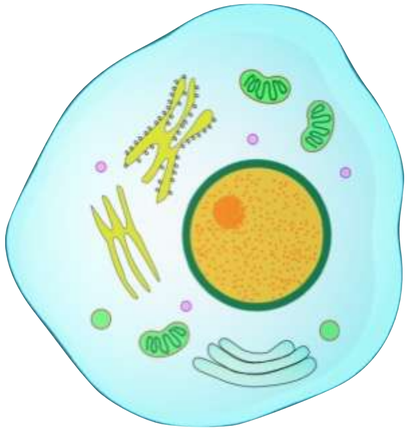
- Average density under certain temperature and pressure conditions
- Hydrogen bonding network
- Diffusion
- Viscosity ….and many more properties….

Study water over certain time (nanosceconds)



Solution of salt/sugar (Solvent)

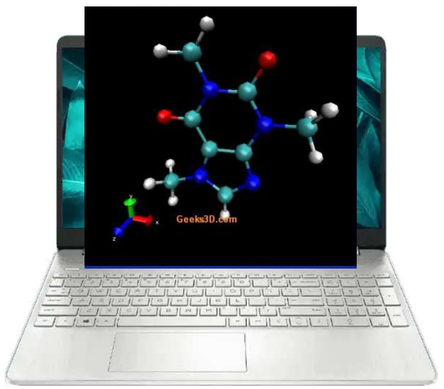
Melting of ice (Phase diagram)



Solvent for biomolecules (Protein folding, ion transport)

D Nayar, C Chakravarty, Phys. Chem. Chem. Phys. 2013, 15, 14162-14177
D Nayar, C Chakravarty Phys. Chem. Chem. Phys. 2014, 16, 10199-10213

The power of computing and technology



Laptop

4-8 CPU cores

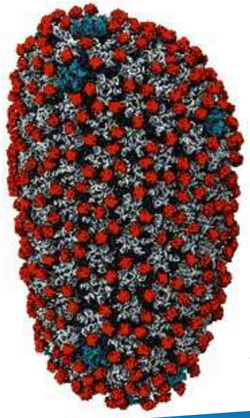
10-100 atoms

Workstation (GPU)

16-150 CPU cores

Approx. 0.1 million atoms

Supercomputer



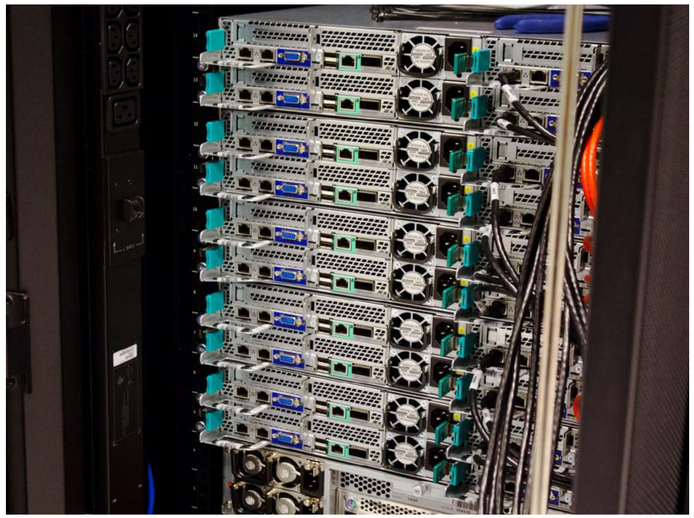
10000-100000 CPU cores

Appox.10 million atoms

http://2017.igem.org/Team:Uppsala/Model

http://www.ks.uiuc.edu/Research/Categories/viruses/spotlight/

Supercomputer



Many efficient computers stacked in a rack and connected by high speed network

A cluster of computers in 2002…

World's fastest supercomputer: *Fugaku,* Japan

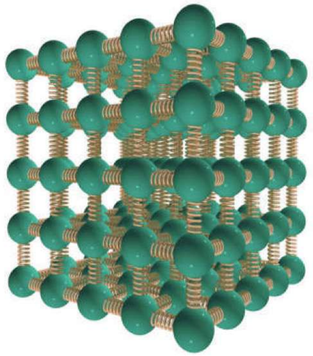
442 PetaFLOPs: can do $442X10^{15}$ operations per second

Google images

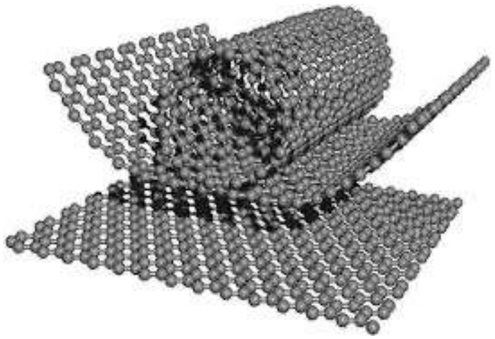
What does computational experiments on Supercomputer enable?

Desipher, Design, Discover, Develop…

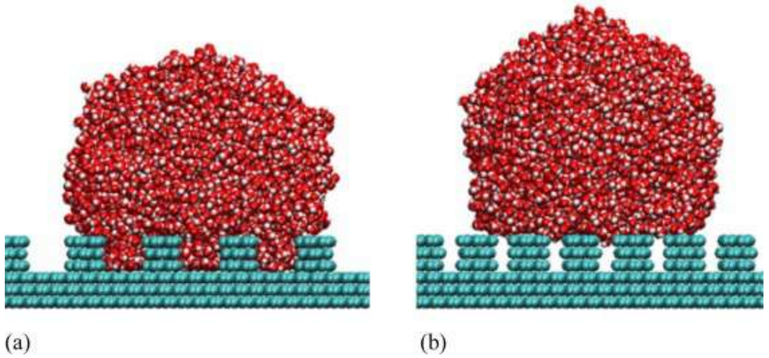
Designing new (nano)materials



Models of crystals

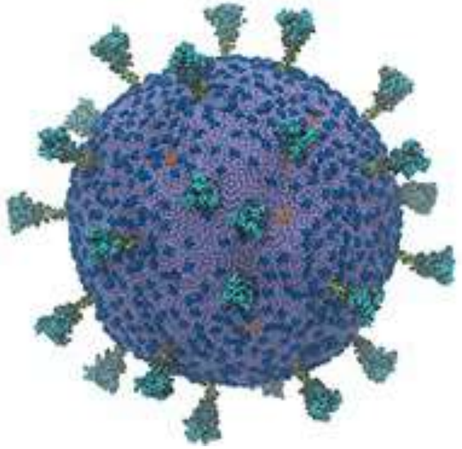


Carbon nanotubes, nanorods, nanosheets

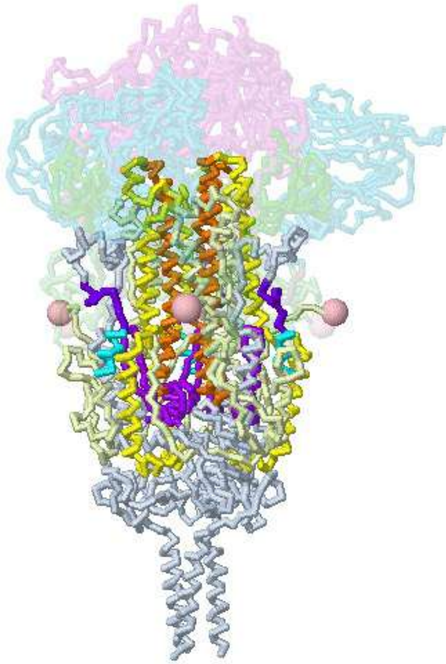


Developing hydrophobic surfaces

Drug design



Corona Virus COVID-19
(Complete virus simulation)



Ultimate challenge:
Simulating the whole living cell
(Trillion atoms!)

Computers & Fluids 2018, 163, 1-6.

https://www.nanowerk.com/nanotechnology/introduction/introduction_to_nanotechnology_22.php

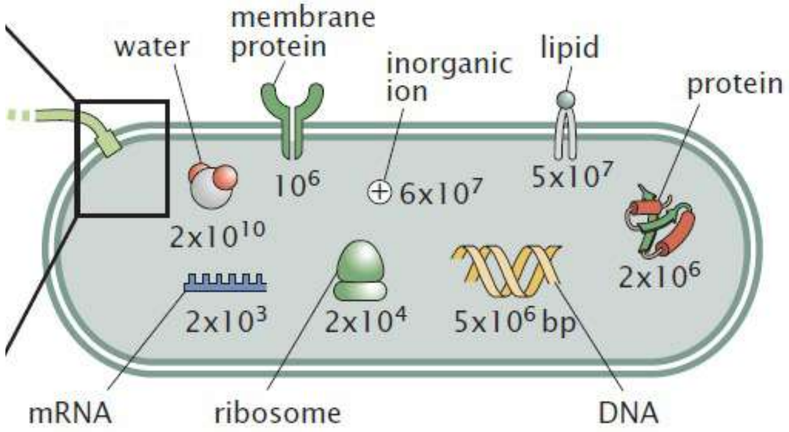
Matter and Interactions, Chabay and Sherwood

Edmond Chow, Georgia Tech

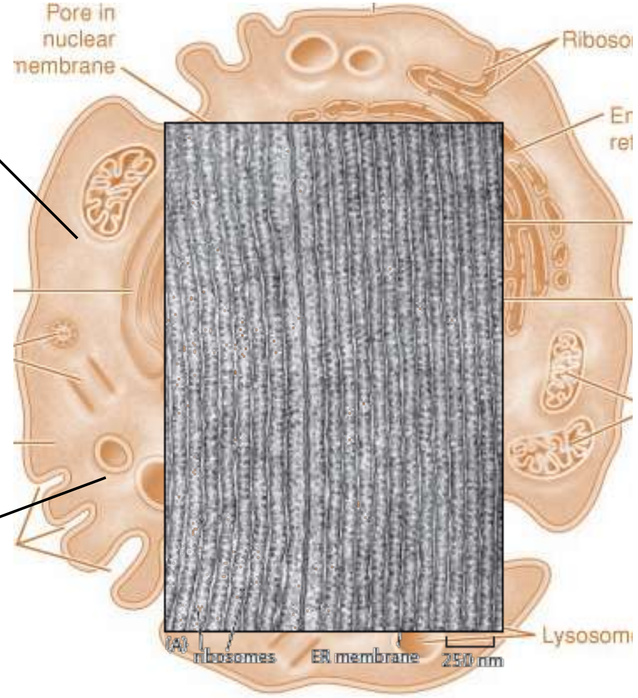
Protopedia

Self assembly: living cell to materials

Research glimpse: Applications of MD simulations in our group

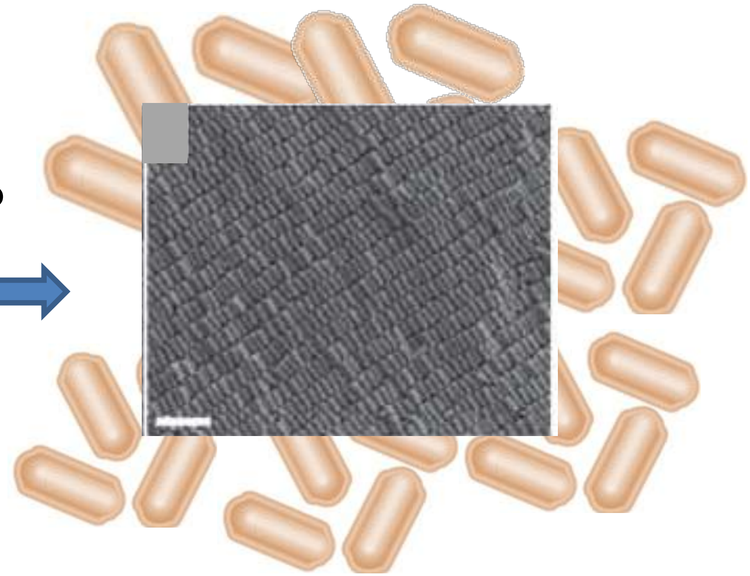


Crowded swimming pool



Physical Biology of Cell, Rob Phillips et al.

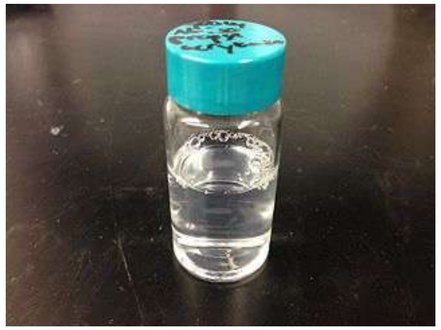
?



J. Mater. Chem. A, 2013, **1**, 2370

Using Nature's design of biological self-assemblies in designing nanomaterials self-assembly!

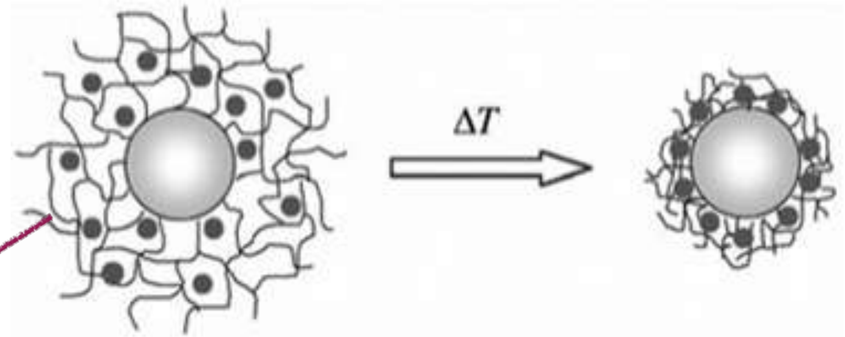
Smart polymers
Why they are smart and how can we design new smart materials?



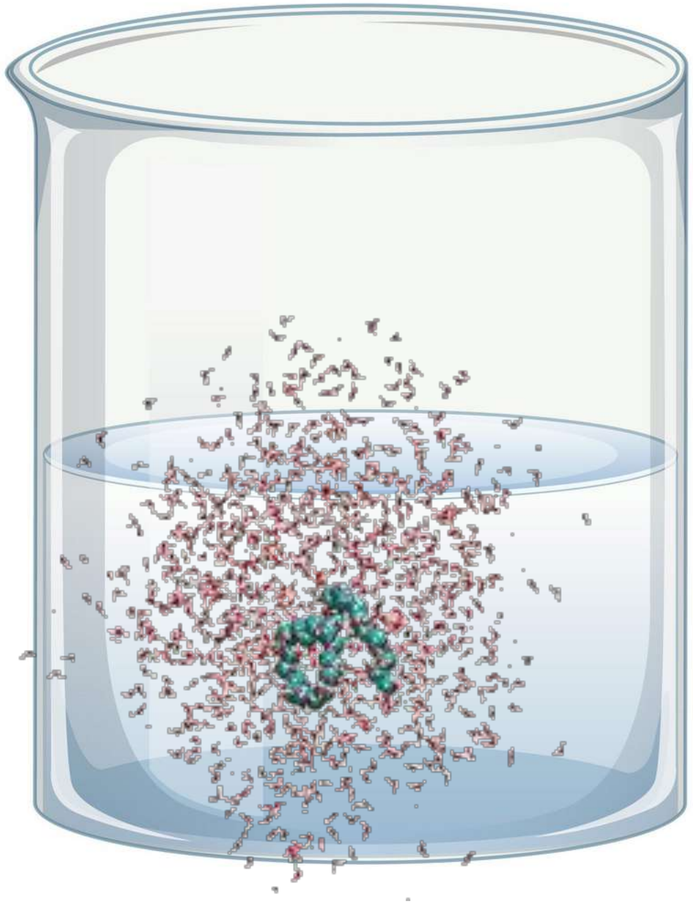
Heating

Cooling

Or chemicals
called osmolytes



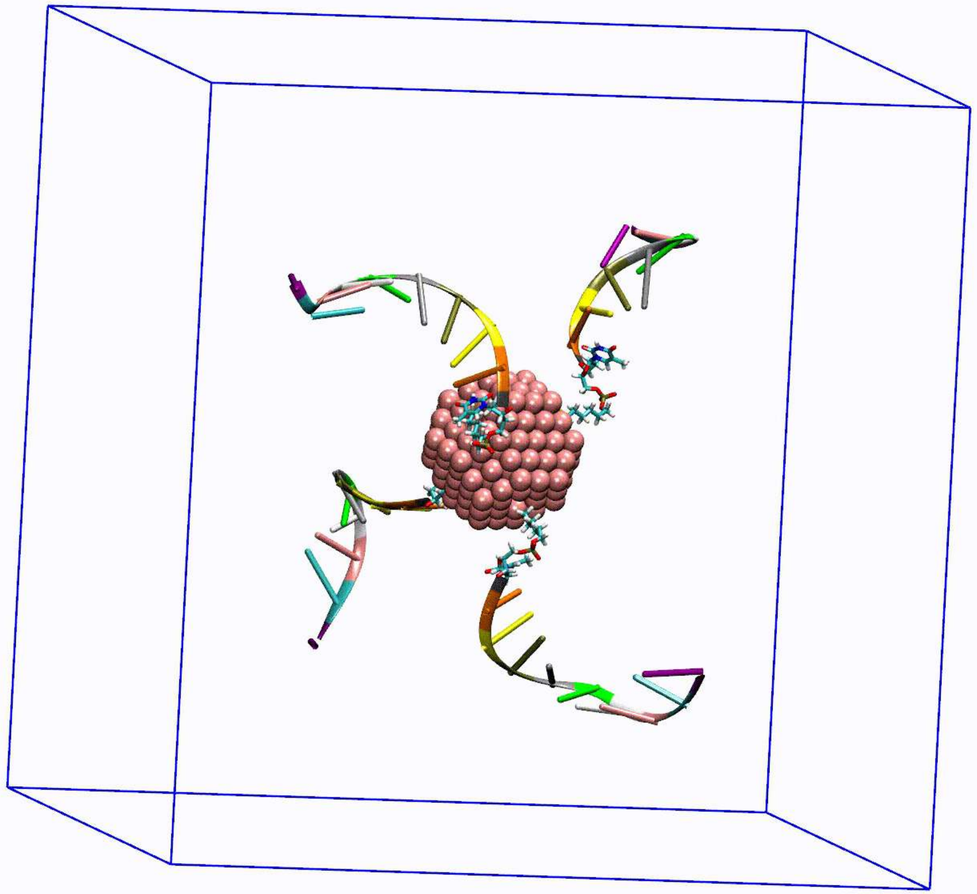
Smart Polymers
(Change their shape and size in response to external stimuli)



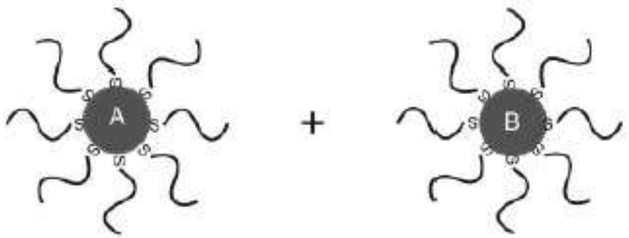
Satyendra Rajput (DN-lab)

D Nayar, NFA van der Vegt, J. Phys. Chem. B 2018, 122, 3587-3595
NFA van der Vegt, D Nayar J. Phys. Chem. B 2017, 121, 9986-9998
D Nayar, Phys. Chem. Chem. Phys. 2020, 22, 18091-18101

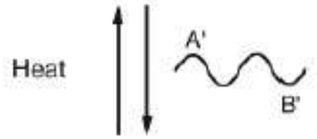
Designing functionalized gold nanoparticle self-assemblies in crowded environment



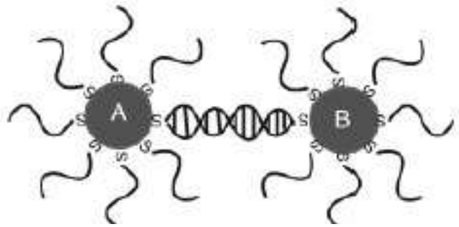
Self-assembled gold nanoparticles find applications in drug delivery and therapeutics



Sharp melting transition



Role of crowding environment ?

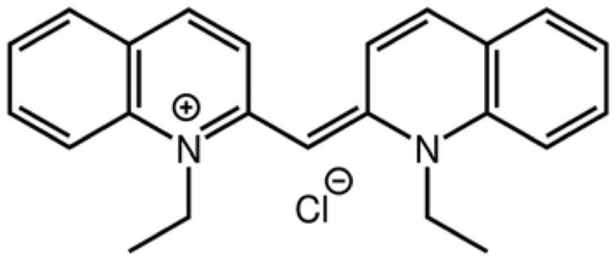


Langmuir 2004**, 20,** 10246

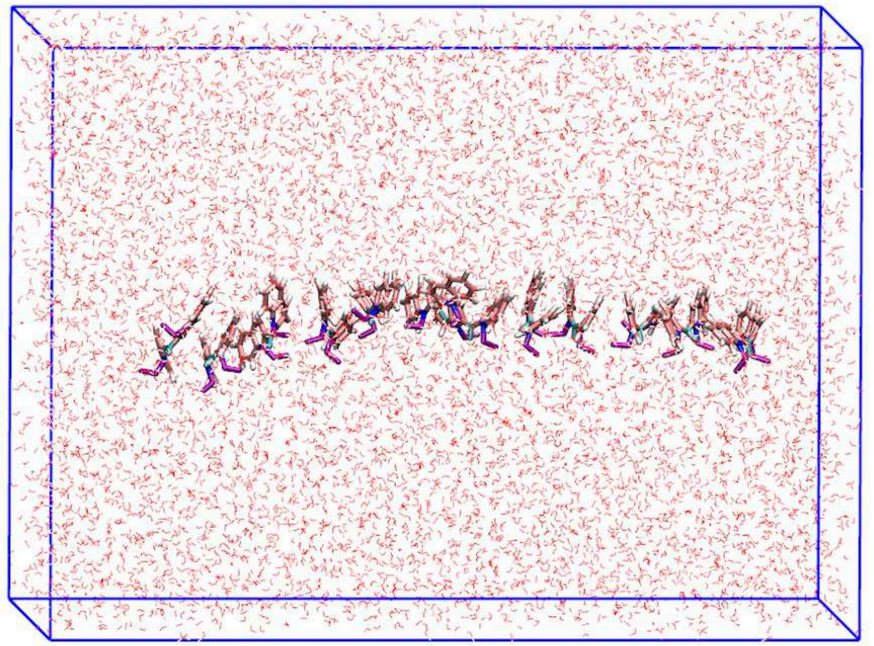
Sibasankar Panigrahy (DN-lab)

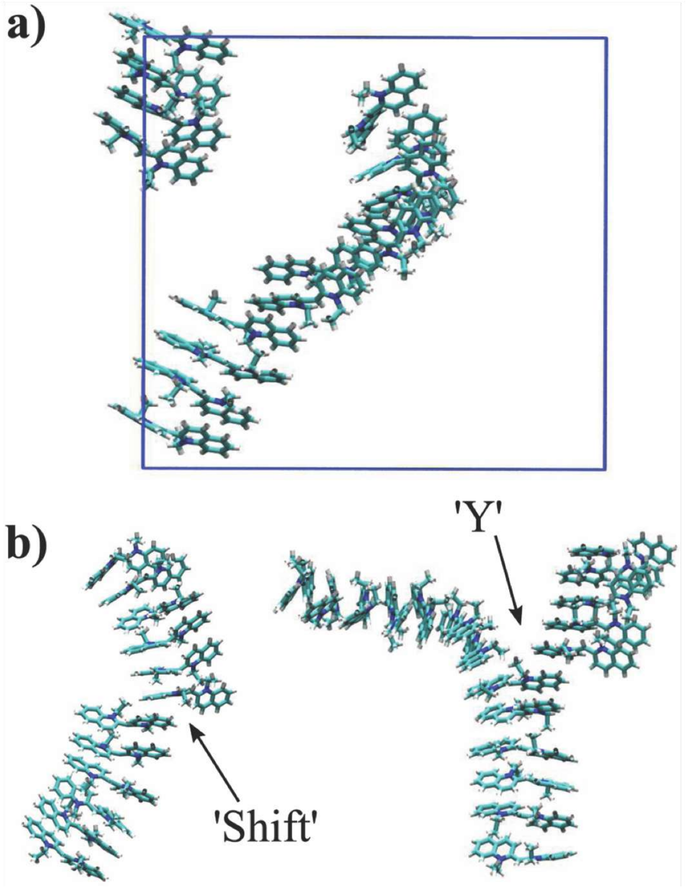
Designing molecular sensors for living cells

Self-assembly of fluorescent dyes



Pseudo isocyanine dye



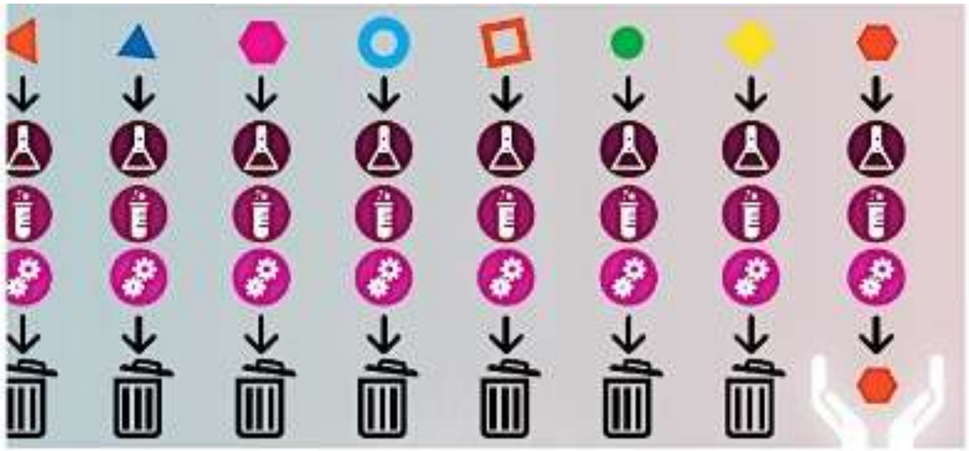


Satyendra Rajput (DN-lab)

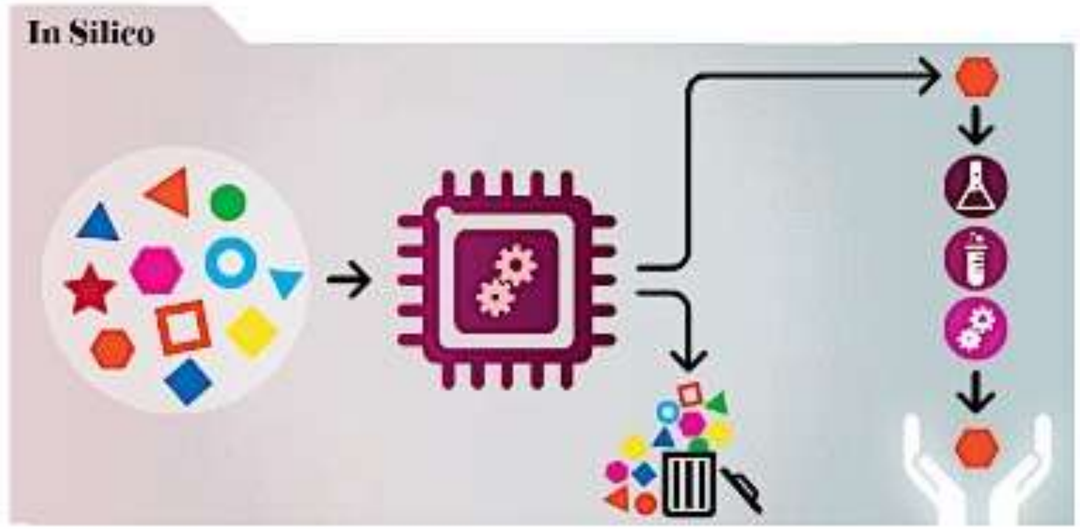
Phys. Chem. Chem. Phys., 2021,**23**, 6408-6421

Artificial Intelligence in Materials Science

Experiments

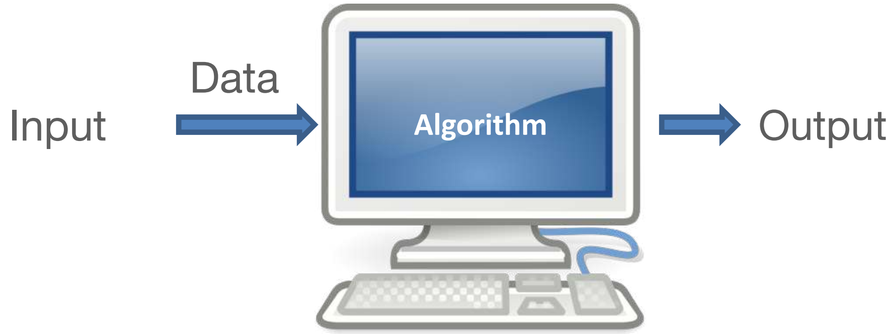


Machine learning

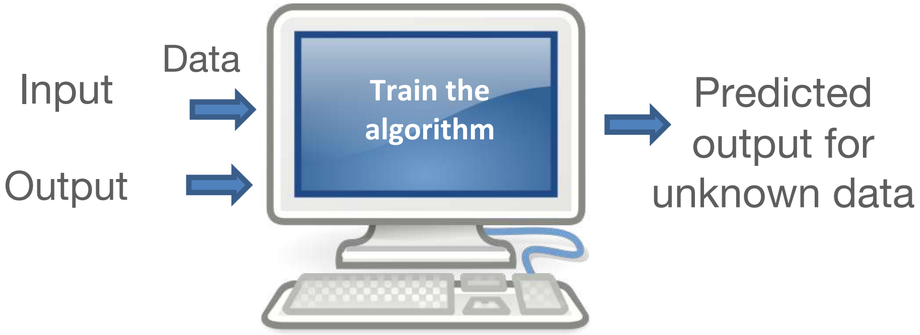


[1] Jain, A., Shin, Y. & Persson, K. A. Computational predictions of energy materials using density functional theory. *Nature Reviews Materials* 1, 15004 (2016).

General Computing



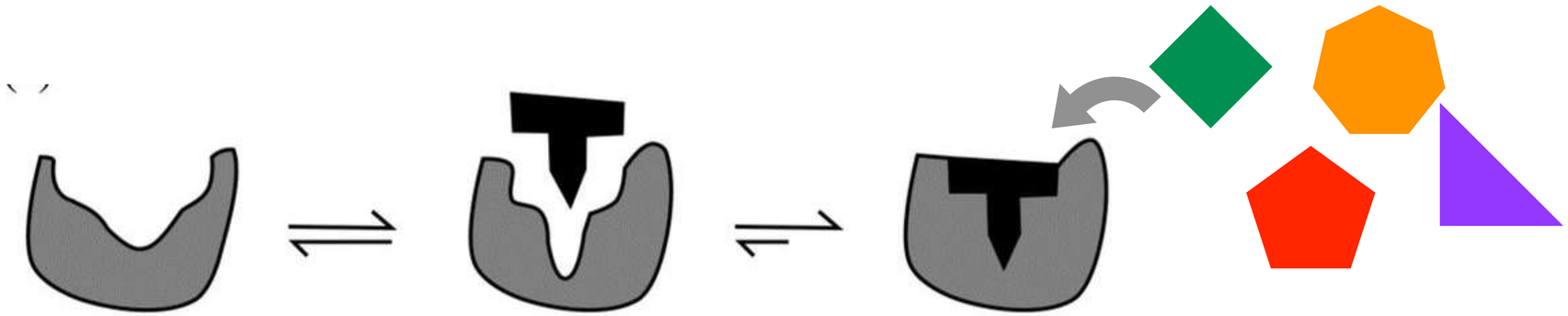
Machine learning



-Materials Discovery
-Materials Design
-Structure-property relationships

Machine Learning for Drug Design:
Generating Ultra-large Datasets for ML models using MD simulation

Which drug molecule can bind to protein to cure the disease?



Protein | **Drug** | **Protein-drug complex**
Binding free energies

Potential drug candidates??

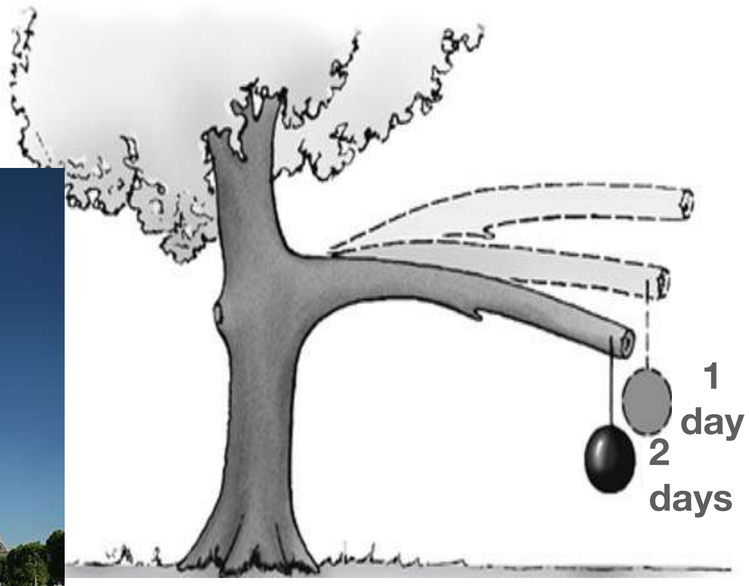
Predict new potential drug candidates

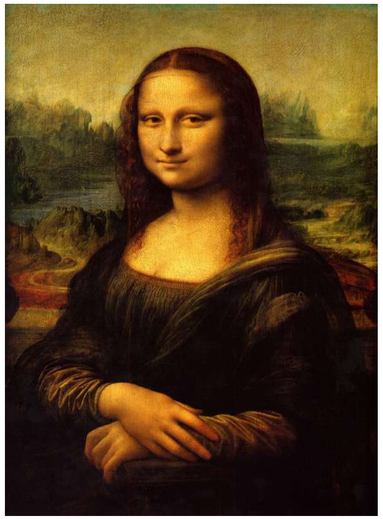
Huge data sets needed for TRAINING and TESTING

20,000 MD simulations !!

DN-lab: In collaboration with *Technology Innovation Hub (TIH) For Data*, *IIIT Hyderabad*

Our journey through the last few weeks…





Some good books to read..

Food for curious minds!

- *Brain: The Story of You (*BBC Documentary also available*)* and *Icognito* by David Eagleman
- *The Double Helix* by James Watson
- *What is Life?* by Erwin Schroedinger
- *Phantoms in the Brain* by V. S. Ramachandran
- *Entropy Demystified* by A. Ben-Naim
- *Surely, You're Joking Mr. Feynman* by Richard P. Feynman
- *The Power of Habit* by Charles Duhigg
- *The New Science of Strong Materials* by J. E. Gordon
- *The Hope Circuit* by Martin Seligman
- *What You can Change and What You Can't* by Martin Seligman

Thank you all for being an awesome and a wonderful class. You have survived the course topics courageously through the online lectures! ☺

Thanks for asking all the interesting questions that helped me in making the lectures more interesting (or were they really interesting!?..).

It has been an amazing experience teaching and interacting with you all !

Keep up the creative spirit, inquisitive energy and the burning curiousity!

All the very best for your future!

Looking forward to working with some of you in near future!