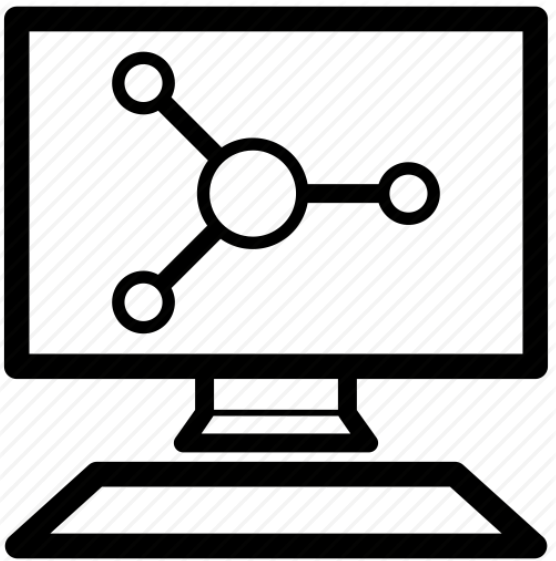
MSE 316 – week 11
Modeling and Simulation in Materials Science and Engineering

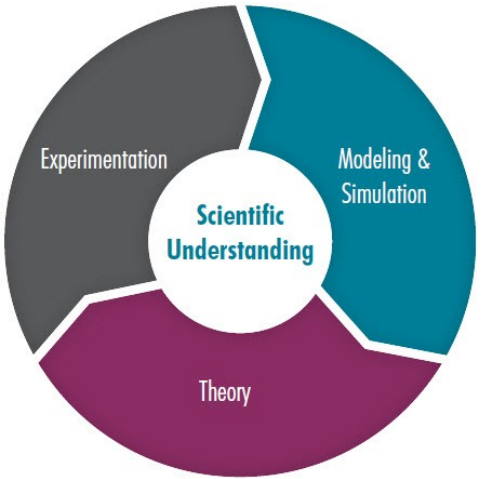
Modelling and Simulation



Modelling and Simulation in MSE

‘Modeling and simulation live at the intersection between theory and experiment.’[1]

Ab initio (or first-principles) methods
Computational methods of physics and chemistry that are based on fundamental physical models and, contrary to empirical methods, do not use experimentally derived parameters except for fundamental physical constants such as speed of light c or Planck constant h.

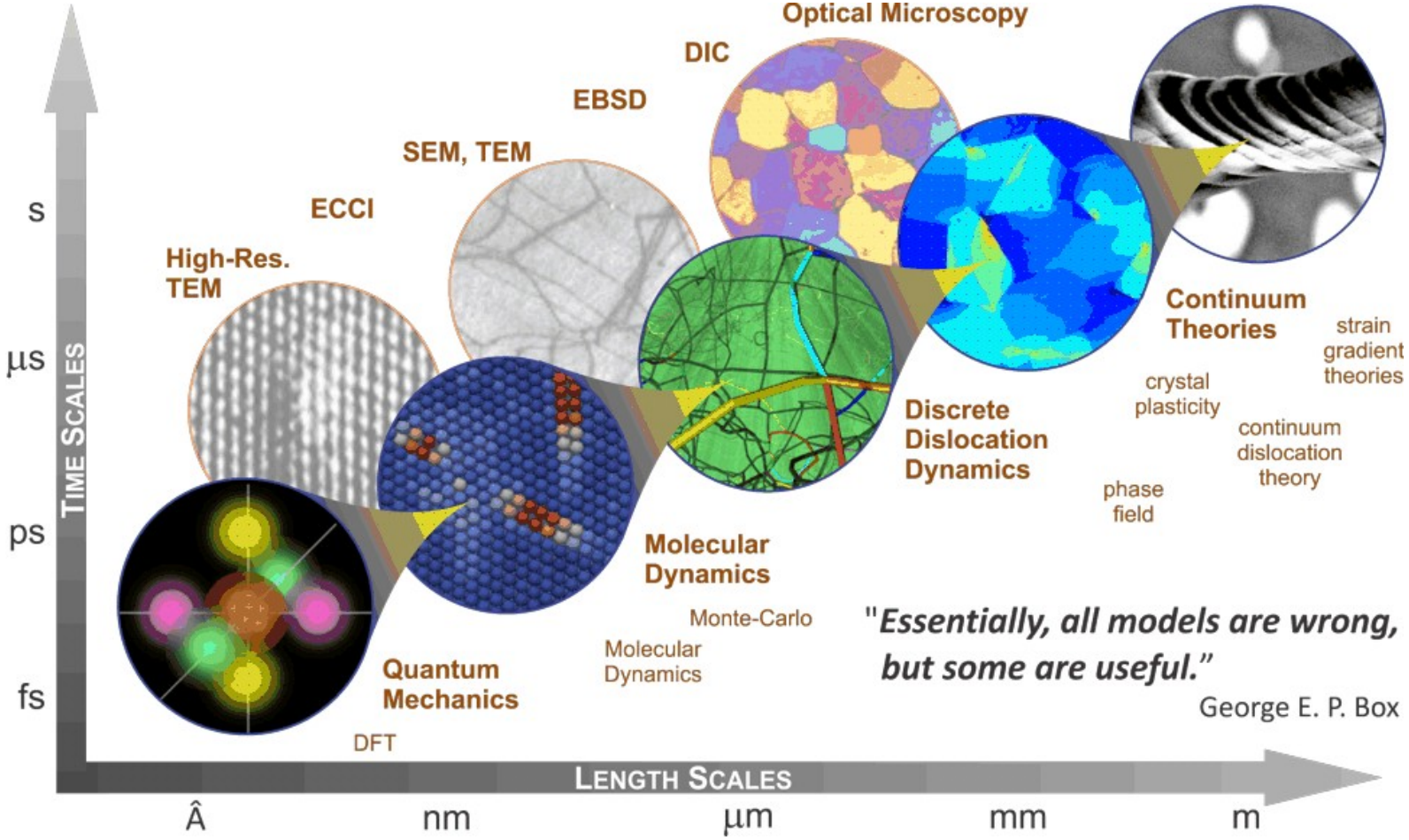


Empirical potential
A certain functional form of the potential energy of a system of interacting atoms with the parameters derived from ab initio calculations and experimental data.

Monte Carlo
A simulation technique for conformational sampling and optimization based on a random search for energetically favourable conformations.

1.https://www.energy.gov/ne/articles/role-modeling-and-simulation-scientific-discovery

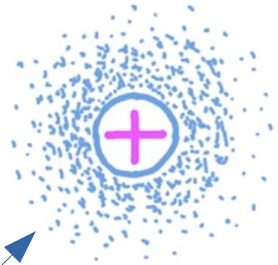
Computational and experimental techniques for a variety of length and time scales



https://mm.ethz.ch/research-overview/coarse-grained-atomistics.html

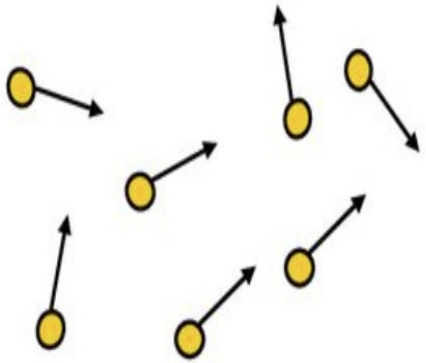
Molecular Dynamics

Newtonian Mechanics



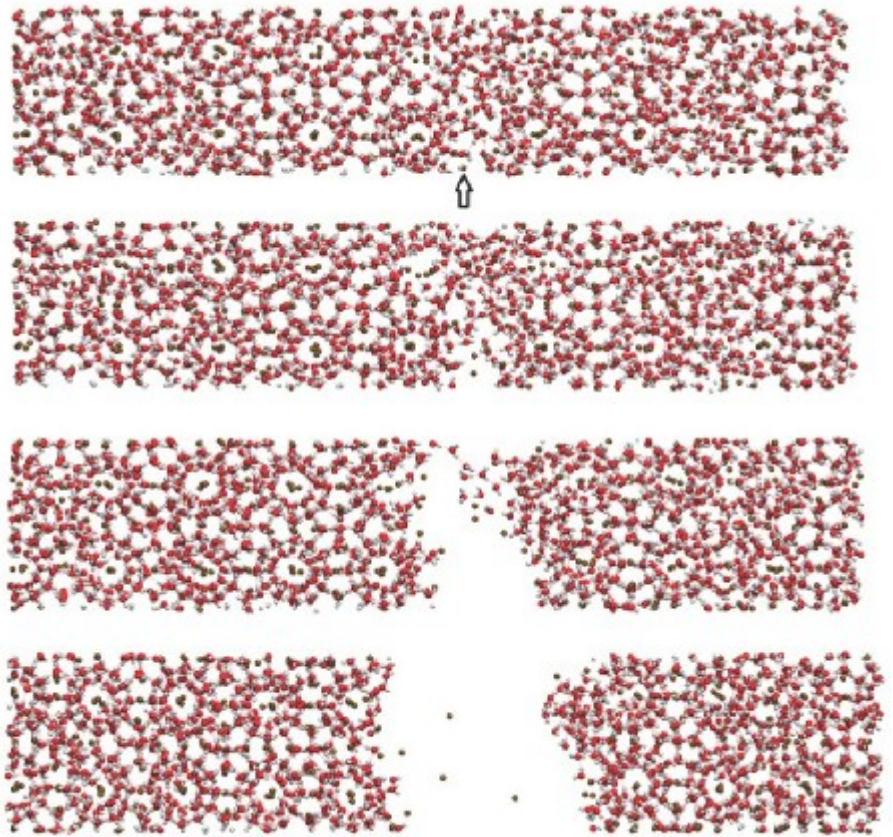
Interatomic potential

-initial velocity
-initial position



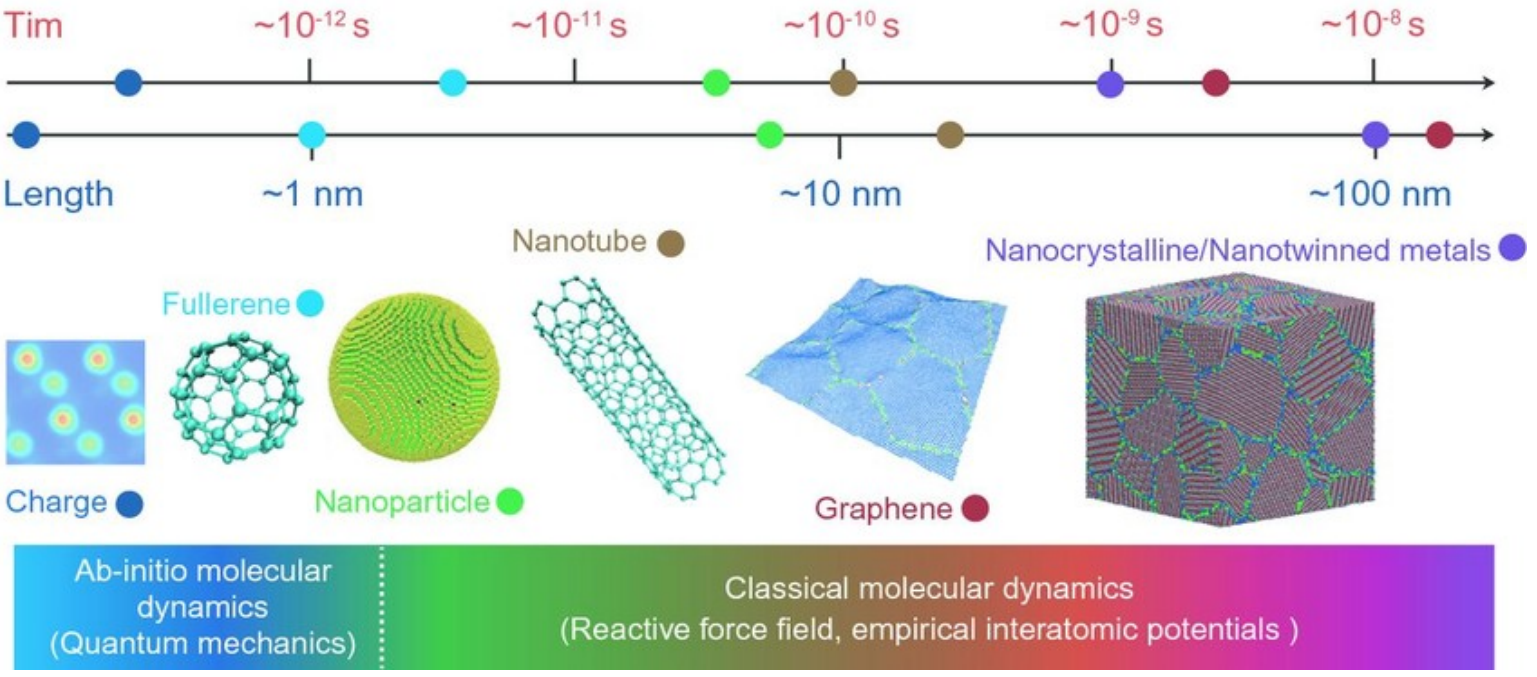
Time evolution of each particle

Molecular dynamics simulation of sI methane hydrate under compression and tension



Wang, Qiang, Tang, Qizhong and Tian, Sen. "Molecular dynamics simulation of sI methane hydrate under compression and tension" Open Chemistry, vol. 18, no. 1, 2020, pp. 69-76

Molecular Dynamics

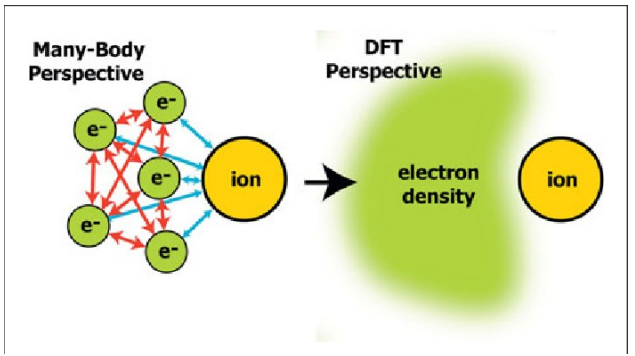


LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator)
S. Plimpton Fast Parallel Algorithms for Short-Range Molecular Dynamics
J. Comput. Phys., 117 (1) (1995), pp. 1-19

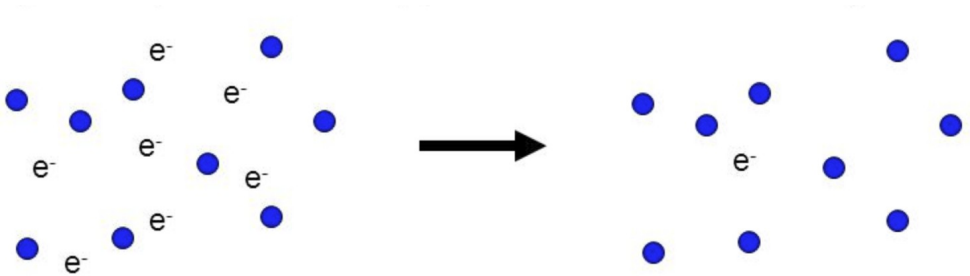
Li, Xiaoyan & Gao, Huajian. (2014). Atomistic modelling of deformation and failure mechanisms in nanostructured materials: Figure 1.. National Science Review. 2. 10.1093/nsr/nwu049.

Density Functional Theory (DFT)

DFT is the most widely used quantum mechanical approximation in solid physics composed of large molecules.



Hohenberg, P. & Kohn, W. Phys. Rev. 136, B864–B871 (1964).



W. Kohn and L. J. Sham Phys. Rev. 140, A1133, 15 November 1965

The Nobel Prize in Chemistry 1998

Photo from the Nobel Foundation archive.
Walter Kohn
Prize share: 1/2

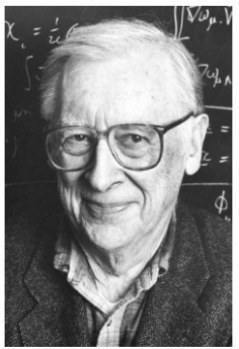


Photo from the Nobel Foundation archive.
John A. Pople
Prize share: 1/2

The Nobel Prize in Chemistry 1998 was divided equally between Walter Kohn "for his development of the density-functional theory" and John A. Pople "for his development of computational methods in quantum chemistry."

Lusk, Mark & Mattsson, Ann. (2011). High-performance computing for materials design to advance energy science. MRS Bulletin. 36. 10.1557/mrs.2011.30.

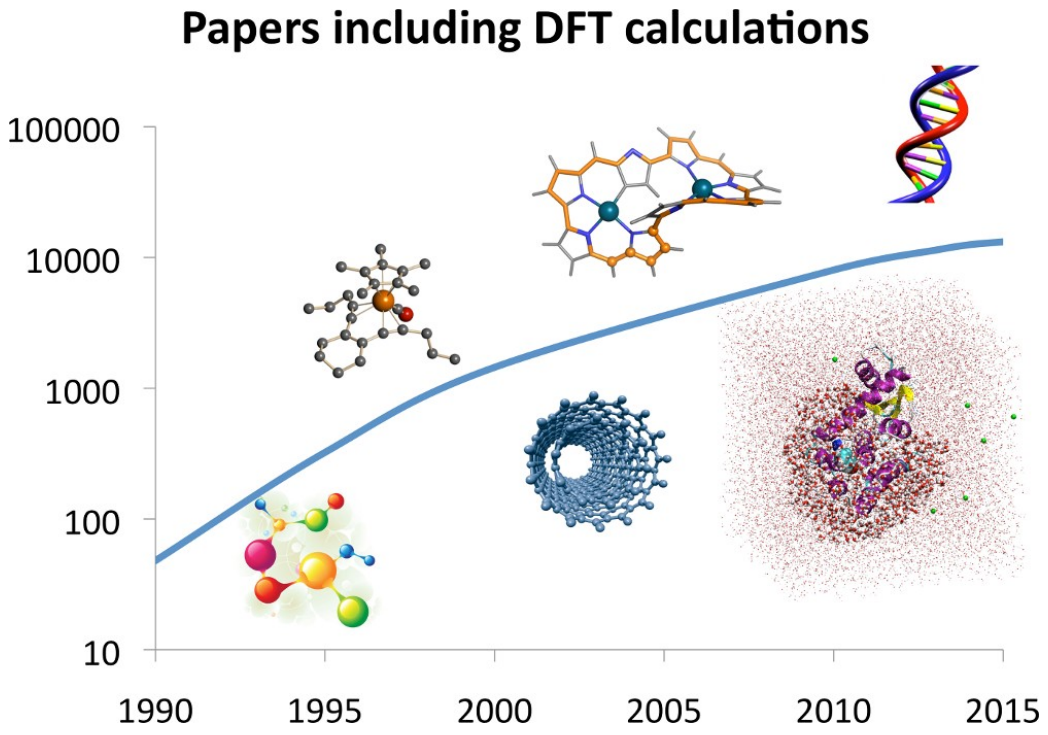
Density Functional Theory (DFT)

Applications

Structure optimization
Drug design
The electronic structure of atoms, molecules and solids
Phonons

Limitations

Not applicable to complex systems, materials



http://dipc.org/internships/2018/DFT_1.html