

Atomic Scale MSE485/CSE485/PHY466
SIMULATION

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Teaching Assistants: ChangMo Yang and Ray Clay

- **Text Book:** *Understanding Molecular Simulation*, by Frenkel and Smit.
- Homepage:
- All information will be conveyed via website.
- **Grading:**
 - (40%) Homework: assigned on web
 - (30%) Exam
 - (30%) Class project: Form in 2-3 person teams. Need “proposal”
- **Computer Needs:**
 - All students can get engineering college and TAUB accounts.
 - PYTHON is the supported language for homework.
- **Introduction to course**
- **Questionnaire**

Introduction to Simulation

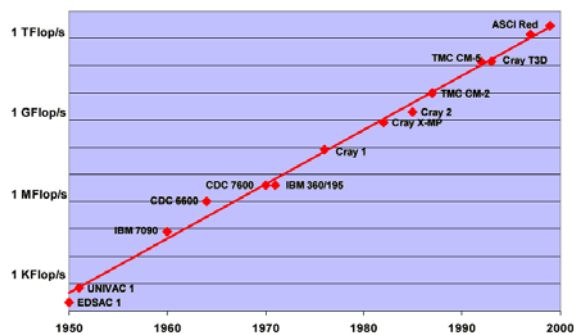
- **Purpose:** Fundamental and rigorous *introduction* to important concepts, techniques, and quantities required for *reliable computer simulation of observables*.
- **Caveats:** cannot cover everything in depth.
 - Must strike a balance (especially with diversity of our class).
- **Why do simulations?**
 - experiments => statistical thermodynamics <== simulations**
- General considerations
- Some history

Why do simulations?

- Simulations are the only general method for “solving” many-body problems.
 - Other methods involve approximations and “experts”.
- Experiment is limited and expensive.
 - Simulations can complement the experiment.
- Simulations are easy even for complex systems.
- Some methods scale up with the computer power which is growing more powerful every year—*Moore’s law*.
- Computational physics *per se* is an interesting and challenging intellectual pursuit (e.g. the fermion sign problem) and a good way to understand the physics.

Moore’s law

- Remarkable 60 year history
- Computer power doubles every 16 months.
- Cost effectiveness also increases



- What does this imply about simulations?
 - Complexity theory gives a way of thinking about it
- Is there a Moore’s law for algorithms and software?
- To keep on track, we need parallel algorithms

Two Simulation Modes

- A. Give us the phenomena and invent a model to mimic the problem. The semi-empirical approach. But one cannot reliably extrapolate the model away from the empirical data.

- B. Maxwell, Boltzmann and Schrödinger gave us the model. All we must do is numerically solve the mathematical problem and determine the properties. (*first-principles or ab initio methods*).

Mode B is what this course is about.

“The general theory of quantum mechanics is now almost complete. The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble.”

Dirac, 1929

Maxwell, Boltzmann and Schrödinger gave us the model (at least for condensed matter physics). Hopefully, all we must do is numerically solve the mathematical problem and determine the properties (using *first principles* or *ab initio methods*).

Without numerical calculations, the predictive power of science is limited. This is what the course is about.

Challenges of Simulation

Physical and mathematical underpinnings:

- What approximations come in?
- Computer time is limited: few particles for short time.
 - Space-Time is 4d.
 - Moore's Law implies lengths and times will double every 6 years if $O(N)$.
- Systems with many particles and long-time scales are problematical.
- Hamiltonian is unknown, until we solve the quantum many-body problem!
- *How do we estimate errors? Statistical and systematic. (bias)*
- How do we manage ever more complex codes?

Complexity

The relationship between time, T , and *degrees of freedom*, N
(for example, the number of atom)

$T \propto O(N)$ linear scaling. Is this the best possible?

$T \propto O(N^3)$ typical in quantum mechanics
(matrix diagonalization, inversion)

$T \propto e^N$ worst case. Quantum dynamics,
direct integrations
("needle in a haystack" multiple minimum)

Estimation of Computer Time and Size

- Today's (~2011) computers, 10^{15} Flops with 3×10^7 s/yr.
 - Hence, $\sim 10^{22}$ Flops/yr are available.
- For $O(N)$ methods, **#ops $\propto N * T * 100$** $\Rightarrow NT \leq 10^{20}$
 (at least 100 factor - 10 neighbors x 10 calculations, say to get distance)
- Simulation box for volume L^3 has ρ (density) N/L^3 , so $N = \rho L^3$.
- Time steps, T , must be proportional to L for information on N atoms to propagate across simulation box, so $T \sim 10 L$. (10 calculations as above).
- Thus $NT = 10 L^4 \leq 10^{20} \Rightarrow L \leq 10^5$ atoms/ side of box.

In Silicon, 10^4 atoms gives $10\mu\text{m}$!

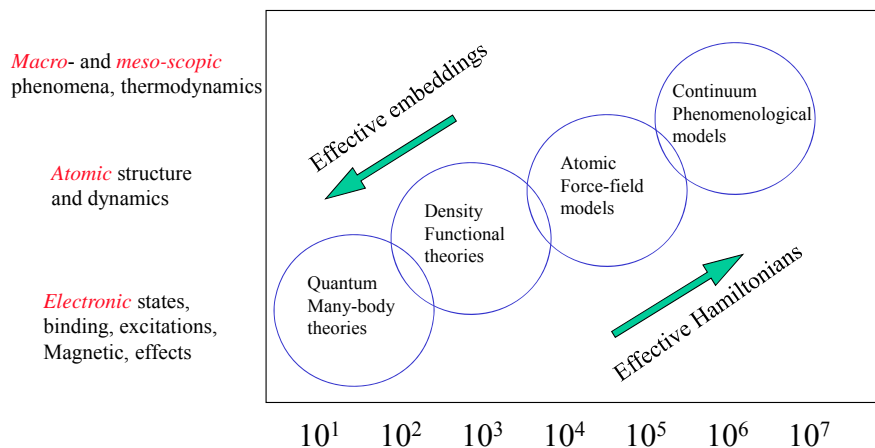
e.g., P.S. Lamdahl *et al.* (1993) did fracture dynamics on 10^8 L-J atoms for 10^8 steps using the CM-5 parallel computer.

SIMULATION CELL IS ALWAYS MICROSCOPIC

We need to approximate macroscale behavior using microscopic information.

Challenges of Simulation

Multi-scale computational materials research:



Short history of Molecular Simulations

- Metropolis, Rosenbluth, Teller (1953) Monte Carlo for hard disks.
- Fermi, Pasta, Ulam (1954) experiment on *ergodicity*
- Alder, Wainwright (1958) liquid-solid transition in hard spheres. “long time tails” (1970)
- Vineyard (1960) Radiation damage using MD
- Rahman (1964) liquid argon, water (1971)
- Verlet (1967) Correlation functions, ...
- Andersen, Rahman, Parrinello (1980) constant pressure MD
- Nose, Hoover, (1983) constant temperature thermostats.
- Car, Parrinello (1985) *ab initio* MD.

Next Lectures

- How to get something from simulations: *statistical errors*
- Review of statistical mechanics
 - *Phase space, Ensembles, Thermodynamic averaging.*
- Newton’s equations and *ergodicity*.
 - *Time averages versus Ensemble averages.*
- Are computer simulations worthwhile?
 - The Fermi-Pasta-Ulam “experiment”
 - Los Alamos report no. LA-1940 (1955).
 - Lectures in Appl. Math 15, 143 (1974).

Homework 1

- Go to calendar page and follow link.
- You must write an elementary error analysis in python. We will cover the material next time.
- On Friday in class we will have a review on python if you need some python help.
- Due Jan. 28
- Hand in the homework even if it is late. But you will not receive full credit if it is late. You need to keep up with the homework!