

1.021, 3.021, 10.333, 22.00 Introduction to Modeling and Simulation
Spring 2011

Part I – Continuum and particle methods

Property calculation I

Lecture 3

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Massachusetts Institute of Technology



Content overview

I. Particle and continuum methods

Lectures 2-13

1. Atoms, molecules, chemistry
2. Continuum modeling approaches and solution approaches
3. Statistical mechanics
4. Molecular dynamics, Monte Carlo
5. Visualization and data analysis
6. Mechanical properties – application: how things fail (and how to prevent it)
7. Multi-scale modeling paradigm
8. Biological systems (simulation in biophysics) – how proteins work and how to model them

II. Quantum mechanical methods

Lectures 14-26

1. It's A Quantum World: The Theory of Quantum Mechanics
2. Quantum Mechanics: Practice Makes Perfect
3. The Many-Body Problem: From Many-Body to Single-Particle
4. Quantum modeling of materials
5. From Atoms to Solids
6. Basic properties of materials
7. Advanced properties of materials
8. What else can we do?

Lecture 3: Property calculation I

Outline:

1. Atomistic model of diffusion
2. Computing power: A perspective
3. How to calculate properties from atomistic simulation
 - 3.1 Thermodynamical ensembles: Micro and macro
 - 3.2 How to calculate properties from atomistic simulation
 - 3.3 How to solve the equations
 - 3.4 Ergodic hypothesis

Goal of today's lecture:

- Exploit Mean Square Displacement function to identify diffusivity, as well as material state & structure
- Provide rigorous basis for property calculation from molecular dynamics simulation results (statistical mechanics)

Additional Reading

Books:

M.J. Buehler (2008): “Atomistic Modeling of Materials Failure”

Allen and Tildesley: “Computer simulation of liquids” (**classic**)

D. C. Rapaport (1996): “The Art of Molecular Dynamics Simulation”

D. Frenkel, B. Smit (2001): “Understanding Molecular Simulation”

J.M. Haile (Wiley, 1992), “Molecular dynamics simulation”

1. Atomistic model of diffusion

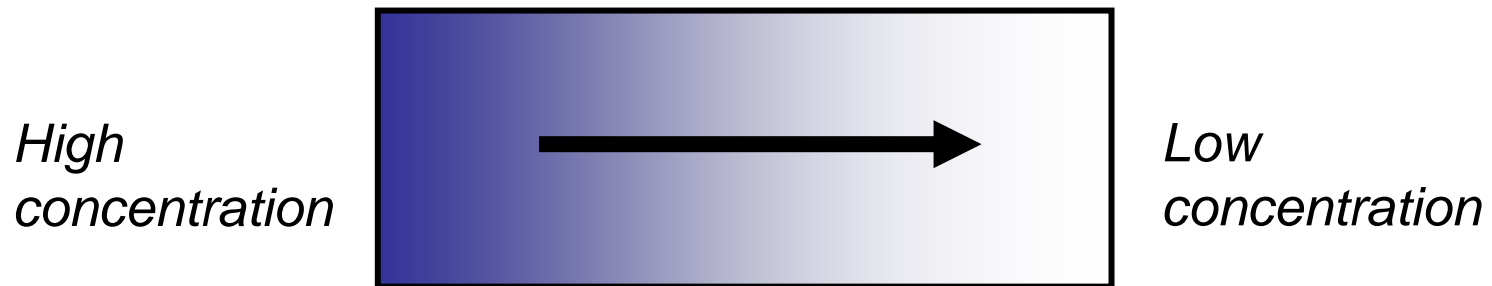
How to build an atomistic bottom-up model to describe the physical phenomena of diffusion?

*Introduce: **Mean Square Displacement***

Recall: Diffusion

- Particles move from a domain with **high concentration** to an area of **low concentration**
- **Macroscopically**, diffusion measured by change in concentration
- **Microscopically**, diffusion is process of spontaneous net movement of particles

Result of random motion of particles (“Brownian motion”)



$$c = m/V = c(\vec{x}, t)$$

Ink droplet in water



hot

cold

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Atomistic description

Back to the **application of diffusion problem...**

- Atomistic description provides alternative way to predict D
- Simple solve equation of motion
- Follow the trajectory of an atom
- Relate the average distance as function of time from initial point to diffusivity

- **Goal: Calculate how particles move “randomly”, away from initial position**

Pseudocode

Set particle positions (e.g. crystal lattice)

Assign initial velocities

For (all time steps):

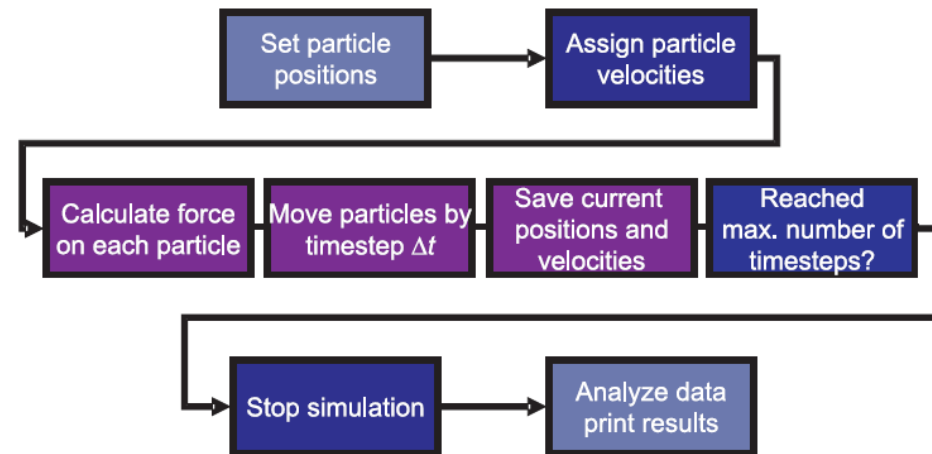
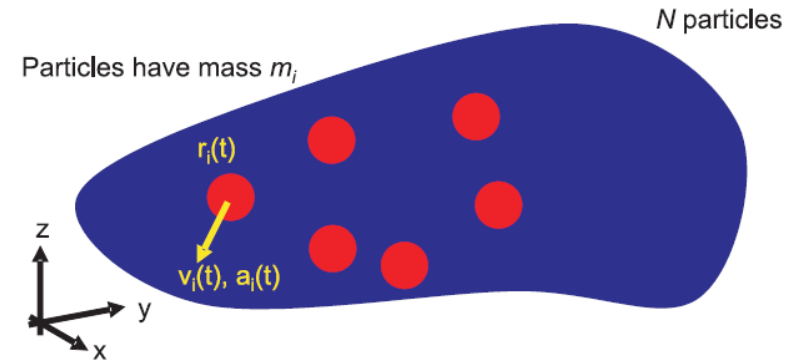
Calculate force on each particle (subroutine)

Move particle by time step Δt

Save particle position, velocity, acceleration

Save results

Stop simulation



$$r_i(t_0 + \Delta t) = \underbrace{2r_i(t_0)}_{\text{Positions at } t_0} - \underbrace{r_i(t_0 - \Delta t)}_{\text{Positions at } t_0 - \Delta t} + \underbrace{a_i(t_0)\Delta t^2}_{\text{Accelerations at } t_0} + \dots$$

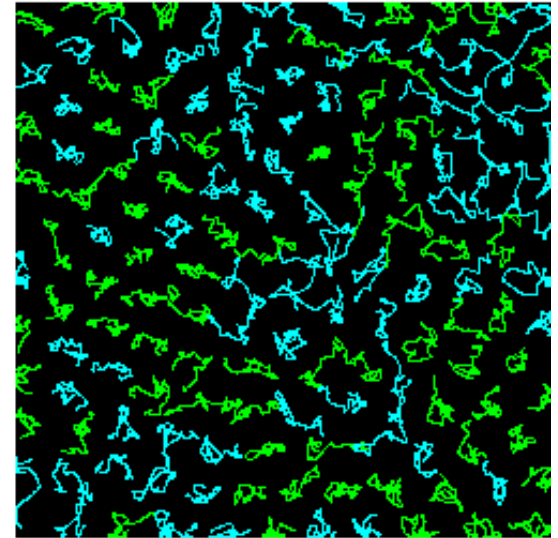
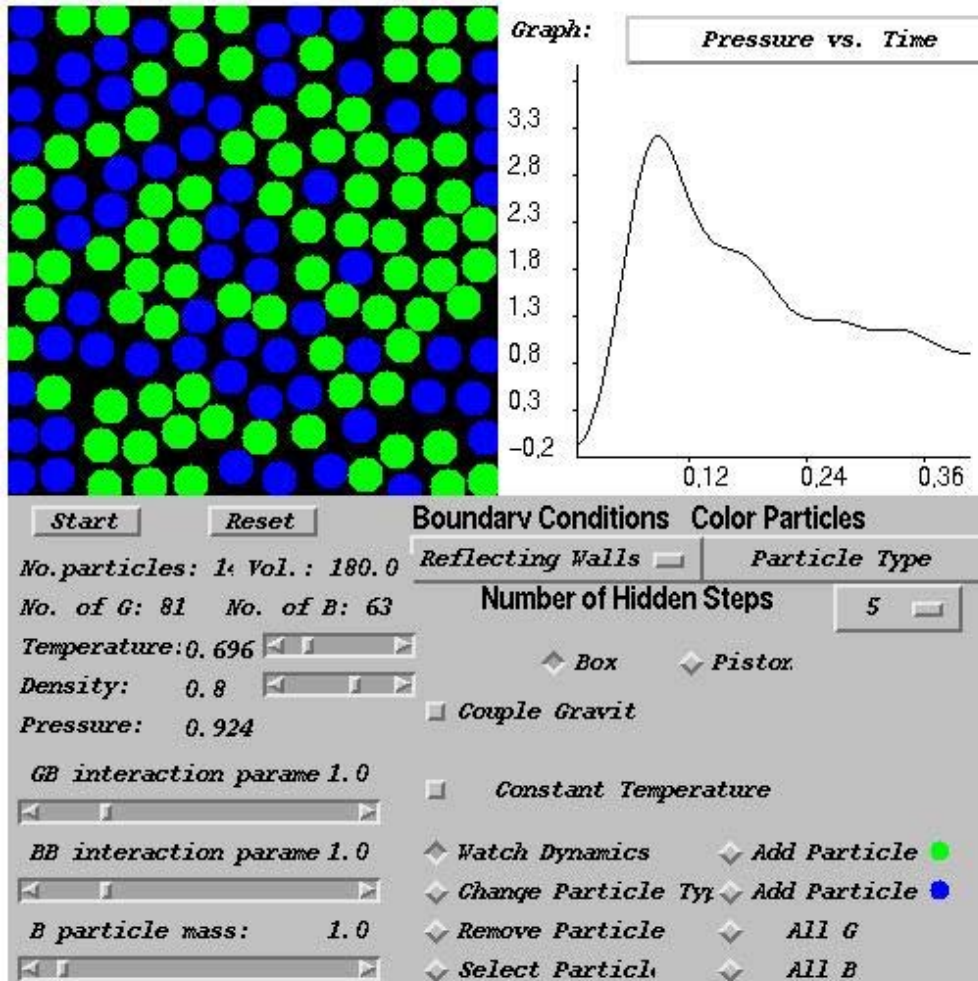
$$a_i = f_i / m$$

Positions
at t_0

Positions
at $t_0 - \Delta t$

Accelerations
at t_0

JAVA applet



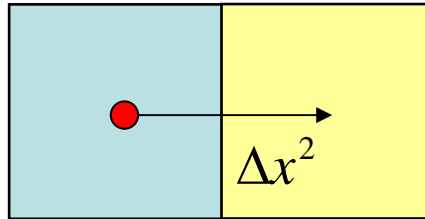
Courtesy of the Center for Polymer Studies at Boston University. Used with permission.

URL <http://polymer.bu.edu/java/java/LJ/index.html>

Link atomistic trajectory with diffusion constant (1D)

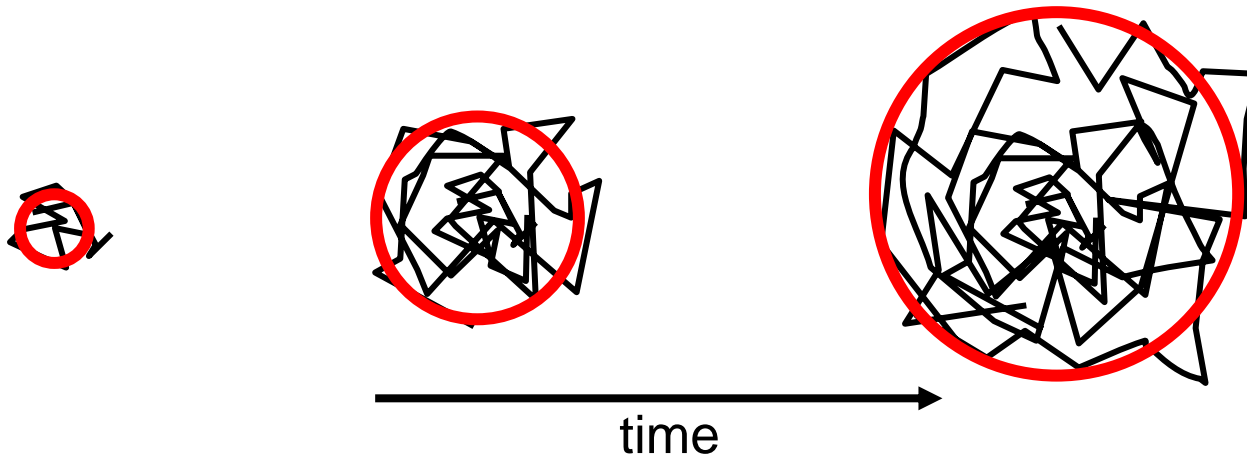
Diffusion constant relates to the “ability” of a particle to move a distance Δx^2 (from left to right) over a time Δt

$$D = p \frac{\Delta x^2}{\Delta t}$$



Idea – Use MD simulation to measure square of displacement from initial position of particles, $\Delta r^2(t)$:

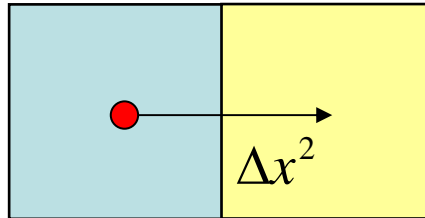
$$\langle \Delta r^2(t) \rangle = \frac{1}{N} \sum_i (\vec{r}_i(t) - \vec{r}_i(t=0))^2 = \frac{1}{N} \sum_i [(\vec{r}_i(t) - \vec{r}_i(t=0)) \cdot (\vec{r}_i(t) - \vec{r}_i(t=0))] \quad \text{scalar product}$$



Link atomistic trajectory with diffusion constant (1D)

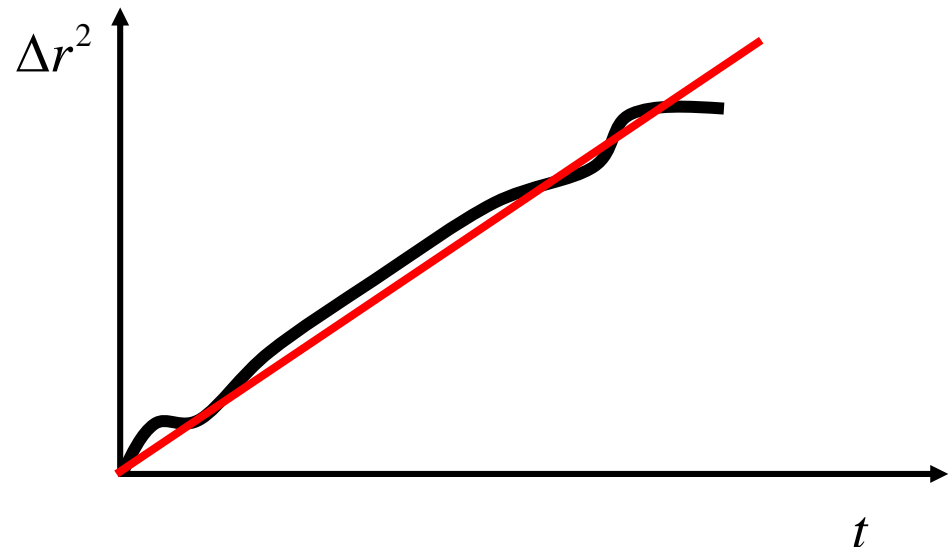
Diffusion constant relates to the “ability” of a particle to move a distance Δx^2 (from left to right) over a time Δt

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MD simulation: Measure square of displacement from initial position of particles, $\Delta r^2(t)$:

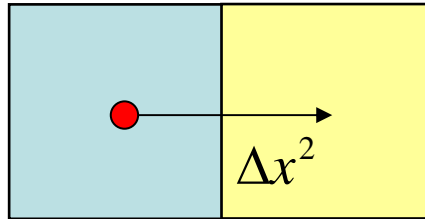
$$\langle \Delta r^2(t) \rangle = \frac{1}{N} \sum_i (\vec{r}_i(t) - \vec{r}_i(t=0))^2$$



Link atomistic trajectory with diffusion constant (1D)

Diffusion constant relates to the “ability” of a particle to move a distance Δx^2 (from left to right) over a time Δt

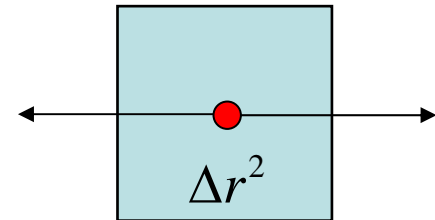
$$D = p \frac{\Delta x^2}{\Delta t}$$



MD simulation: Measure square of displacement from initial position of particles, $\Delta r^2(t)$ and not $\Delta x^2(t)$

Replace

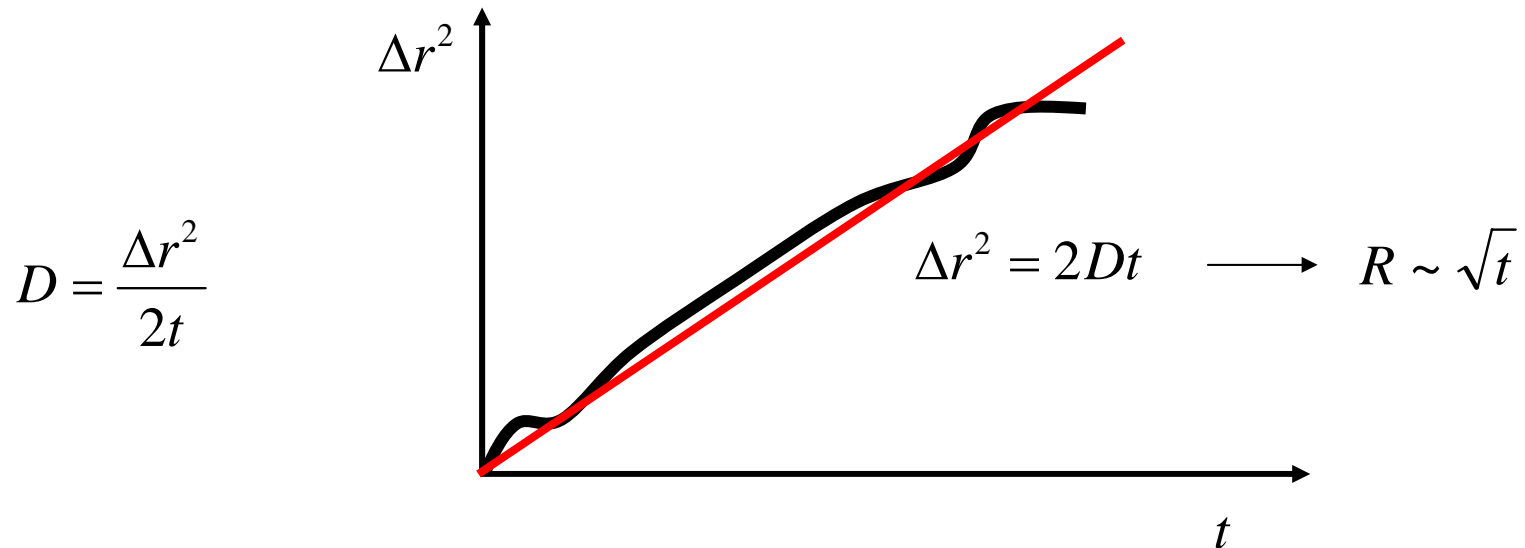
$$D = p \frac{\Delta x^2}{\Delta t} \longrightarrow D = \frac{1}{2} \frac{\Delta r^2}{\Delta t}$$



Factor 1/2 = no directionality in (equal probability to move forth or back)

Link atomistic trajectory with diffusion constant (1D)

MD simulation: Measure square of displacement from initial position of particles, $\Delta r^2(t)$:



Link atomistic trajectory with diffusion constant (2D/3D)

$$D = p \frac{\Delta x^2}{\Delta t}$$



Higher dimensions

$$D = \frac{1}{2} \frac{1}{d} \frac{\Delta r^2}{\Delta t}$$

Factor 1/2 = no directionality in (forth/back)

Factor $d = 1, 2, \text{ or } 3$ due to 1D, 2D, 3D (dimensionality)

Since:

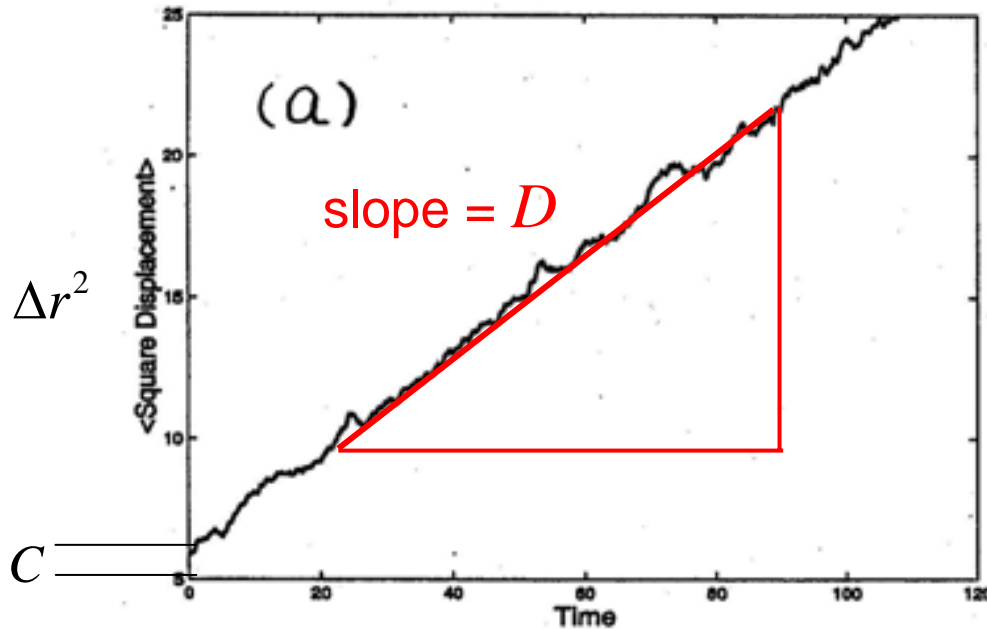
$$2dD\Delta t \sim \Delta r^2$$

$$2dD\Delta t + C = \Delta r^2$$

$C = \text{constant}$ (does not affect D)

Example: MD simulation

Mean Square Displacement function



Courtesy of Sid Yip. Used with permission.

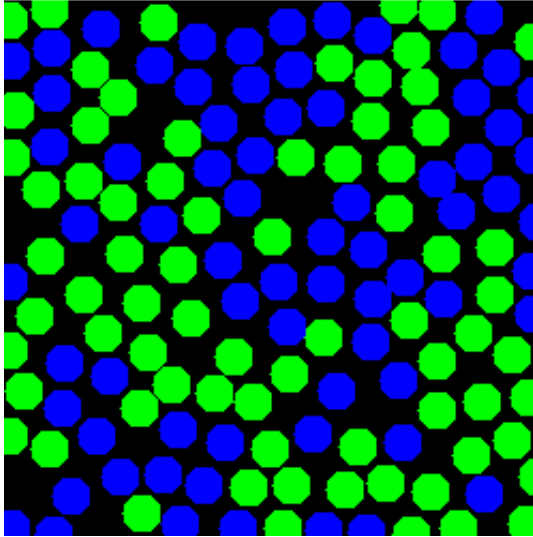
$$D = \frac{1}{2d} \lim_{t \rightarrow \infty} \frac{d}{dt} \langle \Delta r^2 \rangle$$

↑
1D=1, 2D=2, 3D=3

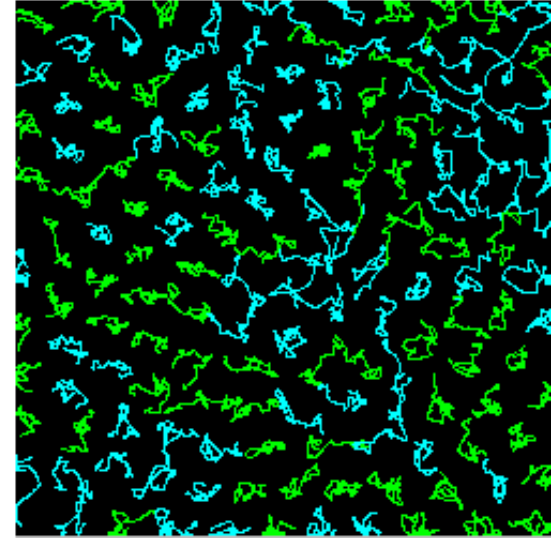
$$D = \frac{1}{2d} \lim_{t \rightarrow \infty} \frac{d}{dt} \langle \Delta r^2 \rangle$$

$\langle .. \rangle$ = average over all particles

Example molecular dynamics



Particles

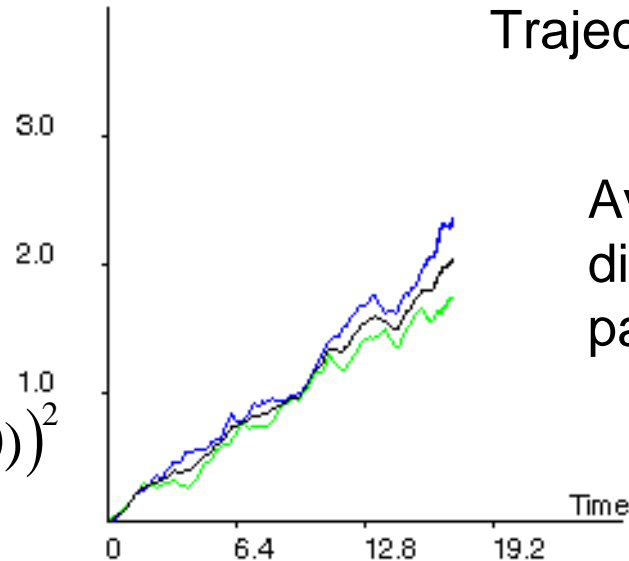


Trajectories

**Mean Square
Displacement function**

$$\langle \Delta r^2(t) \rangle = \frac{1}{N} \sum_i (\vec{r}_i(t) - \vec{r}_i(t=0))^2$$

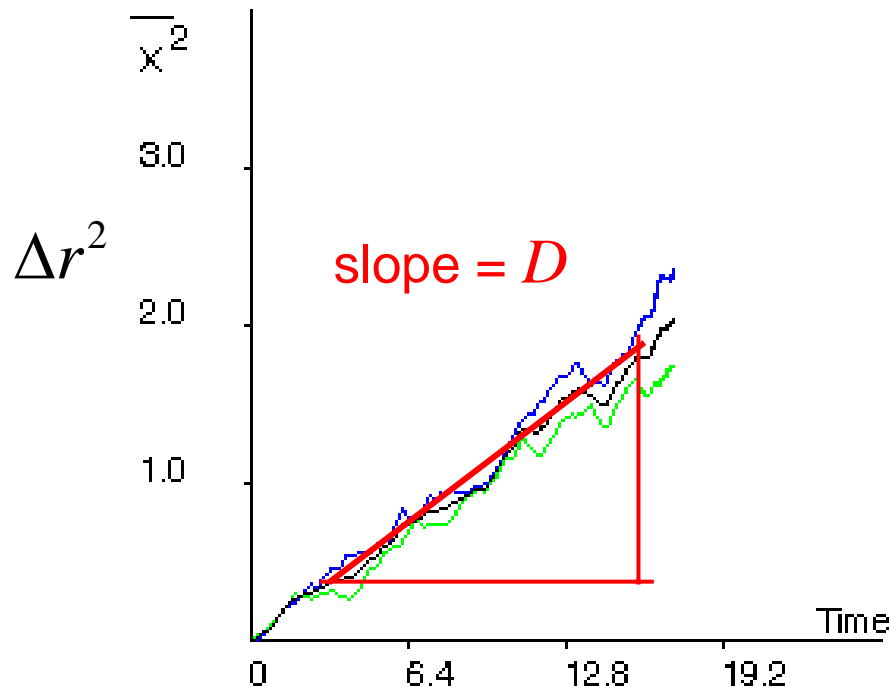
Δr^2



Average square of
displacement of all
particles

Example calculation of diffusion coefficient

$$\langle \Delta r^2(t) \rangle = \frac{1}{N} \sum_i \underbrace{(r_i(t))}_{\text{Position of atom } i \text{ at time } t} - \underbrace{r_i(t=0)}_{\text{Position of atom } i \text{ at time } t=0}$$

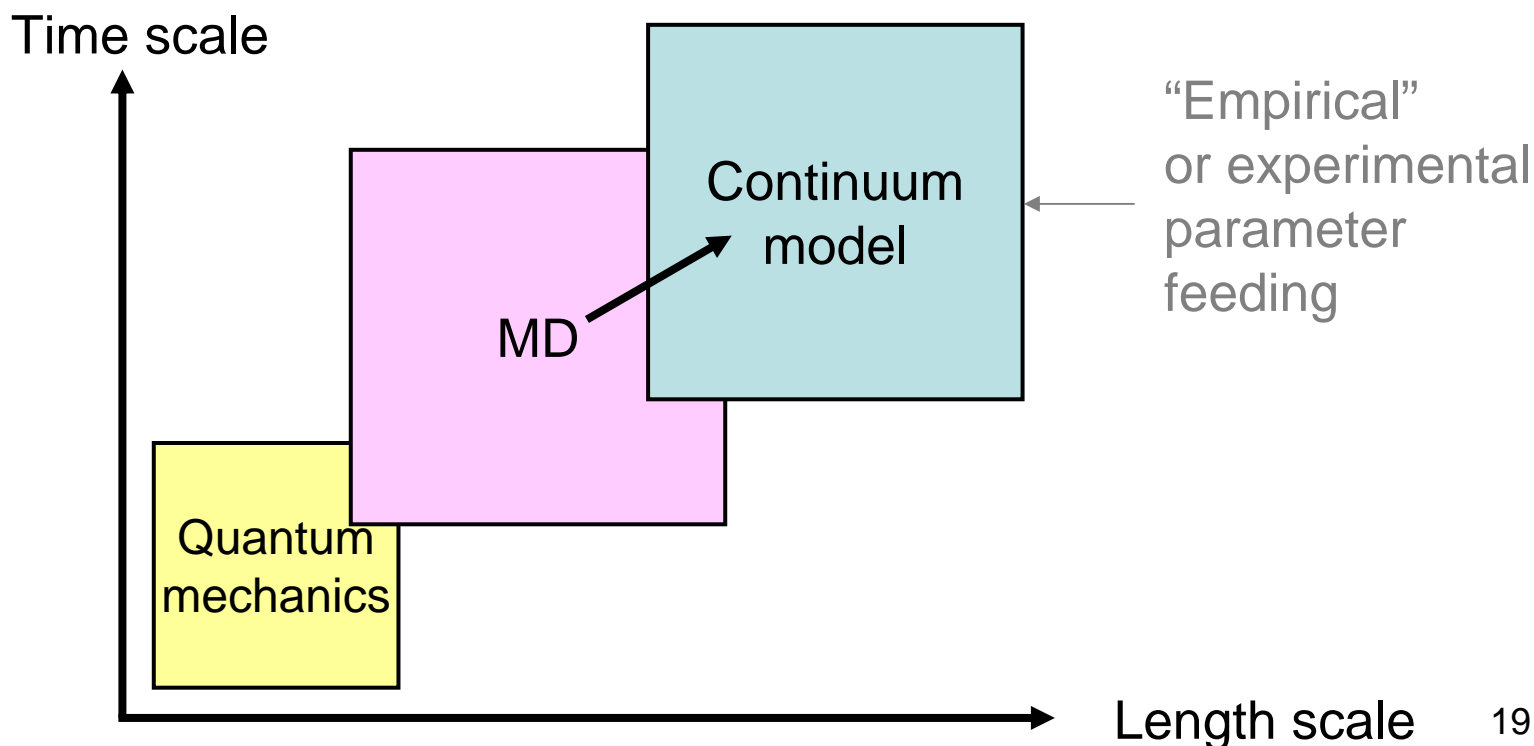


$$D = \frac{1}{2d} \lim_{t \rightarrow \infty} \frac{d}{dt} \langle \Delta r^2 \rangle$$

↑
1D=1, 2D=2, 3D=3

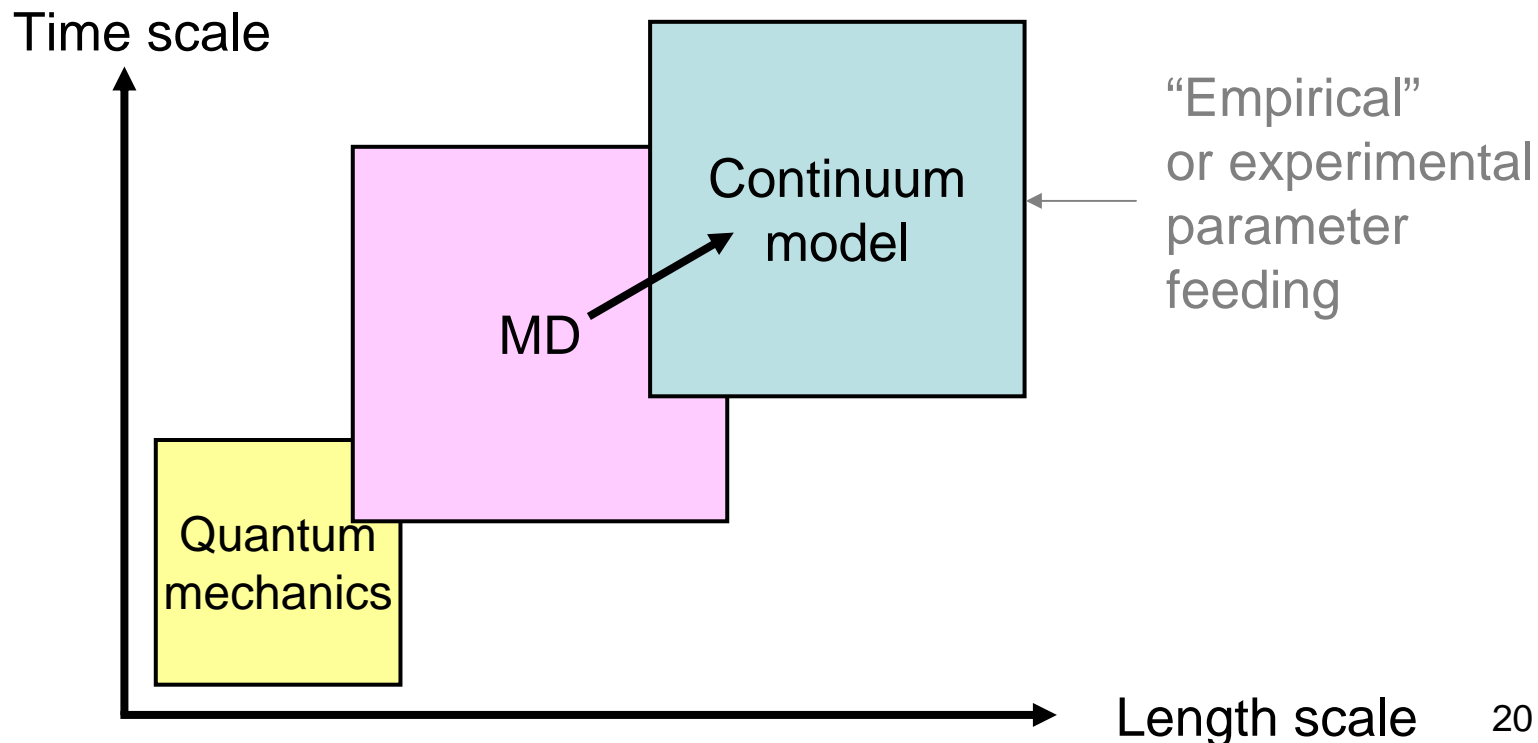
Summary

- Molecular dynamics provides a powerful approach to relate the diffusion constant that appears in continuum models to atomistic trajectories
- Outlines multi-scale approach: Feed parameters from atomistic simulations to continuum models



Summary

- Molecular dynamics provides a powerful approach to relate the diffusion constant that appears in continuum models to atomistic trajectories
- Outlines multi-scale approach: Feed parameters from atomistic simulations to continuum models



MD modeling of crystals – solid, liquid, gas phase

- Crystals: Regular, ordered structure
- The corresponding particle motions are small-amplitude vibrations about the lattice site, diffusive movements over a local region, and long free flights interrupted by a collision every now and then.
- Liquids: Particles follow Brownian motion (collisions)
- Gas: Very long free paths

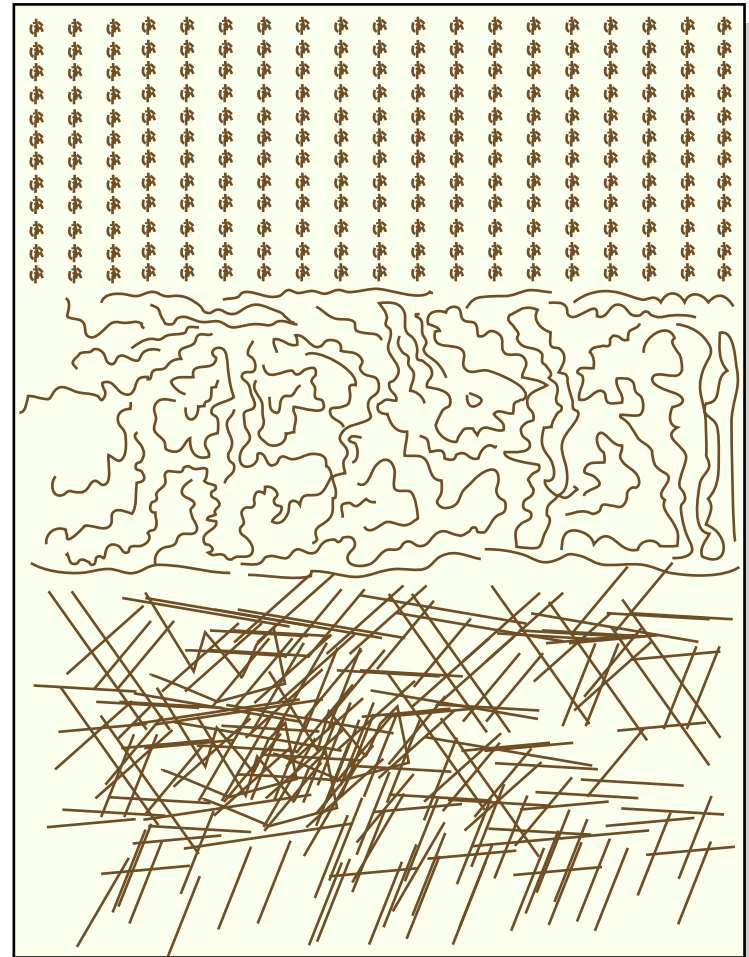
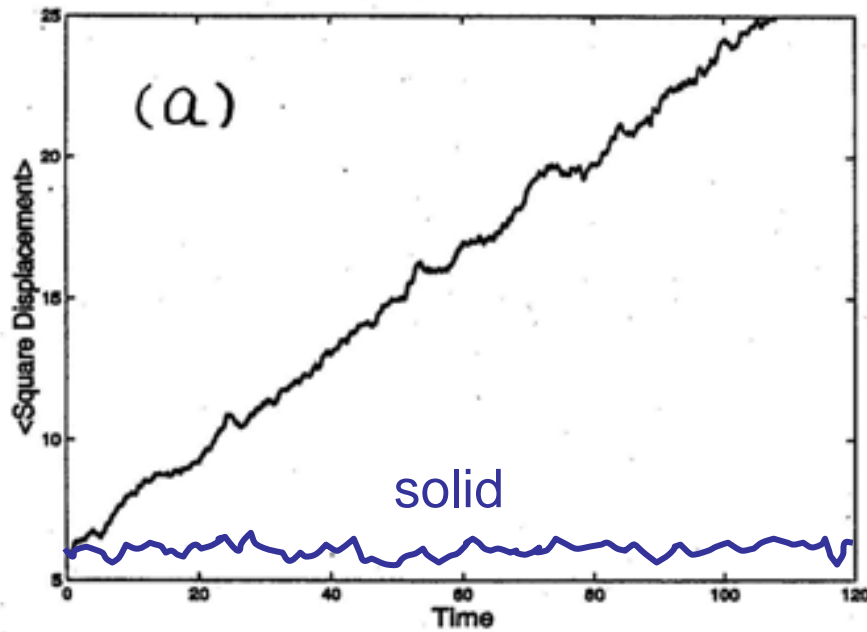


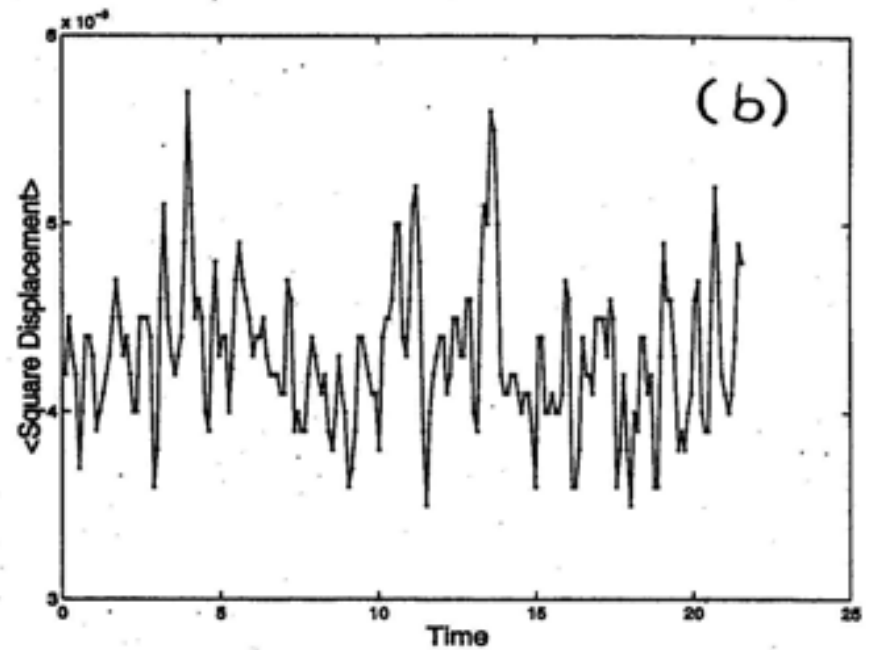
Image by MIT OpenCourseWare. After J. A. Barker and D. Henderson.

Example: MD simulation results

liquid

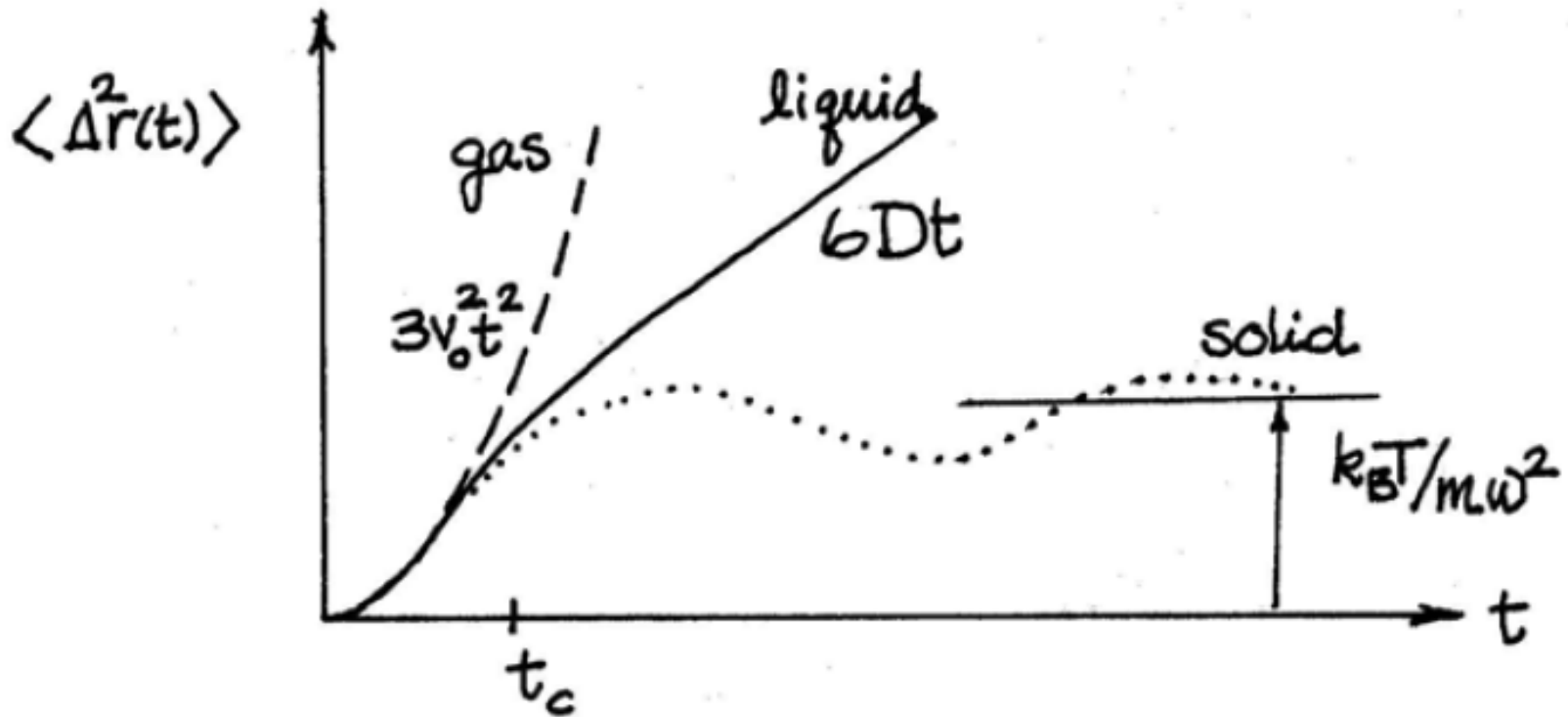


solid



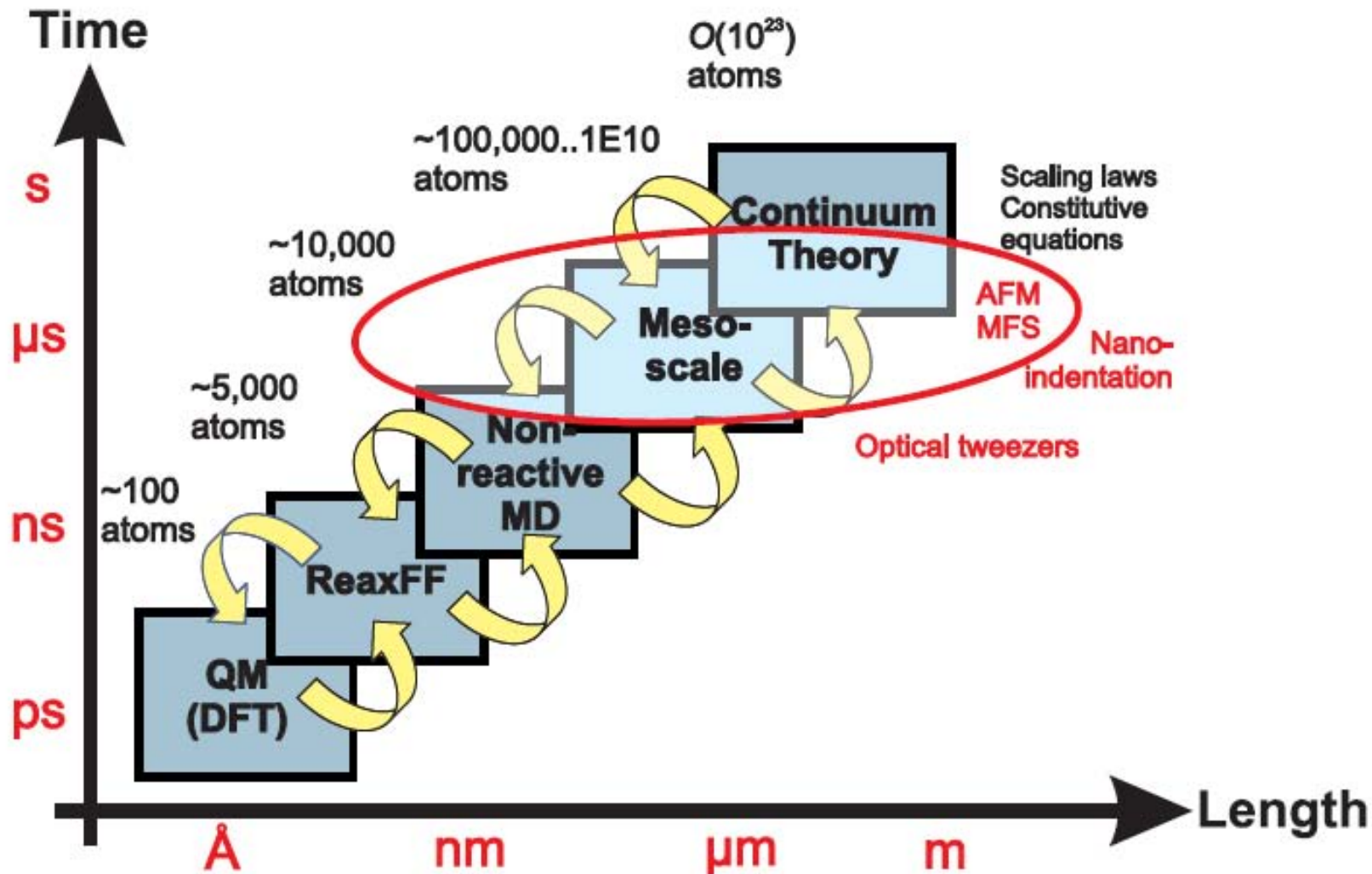
Courtesy of Sid Yip. Used with permission.

Atomistic trajectory



Courtesy of Sid Yip. Used with permission.

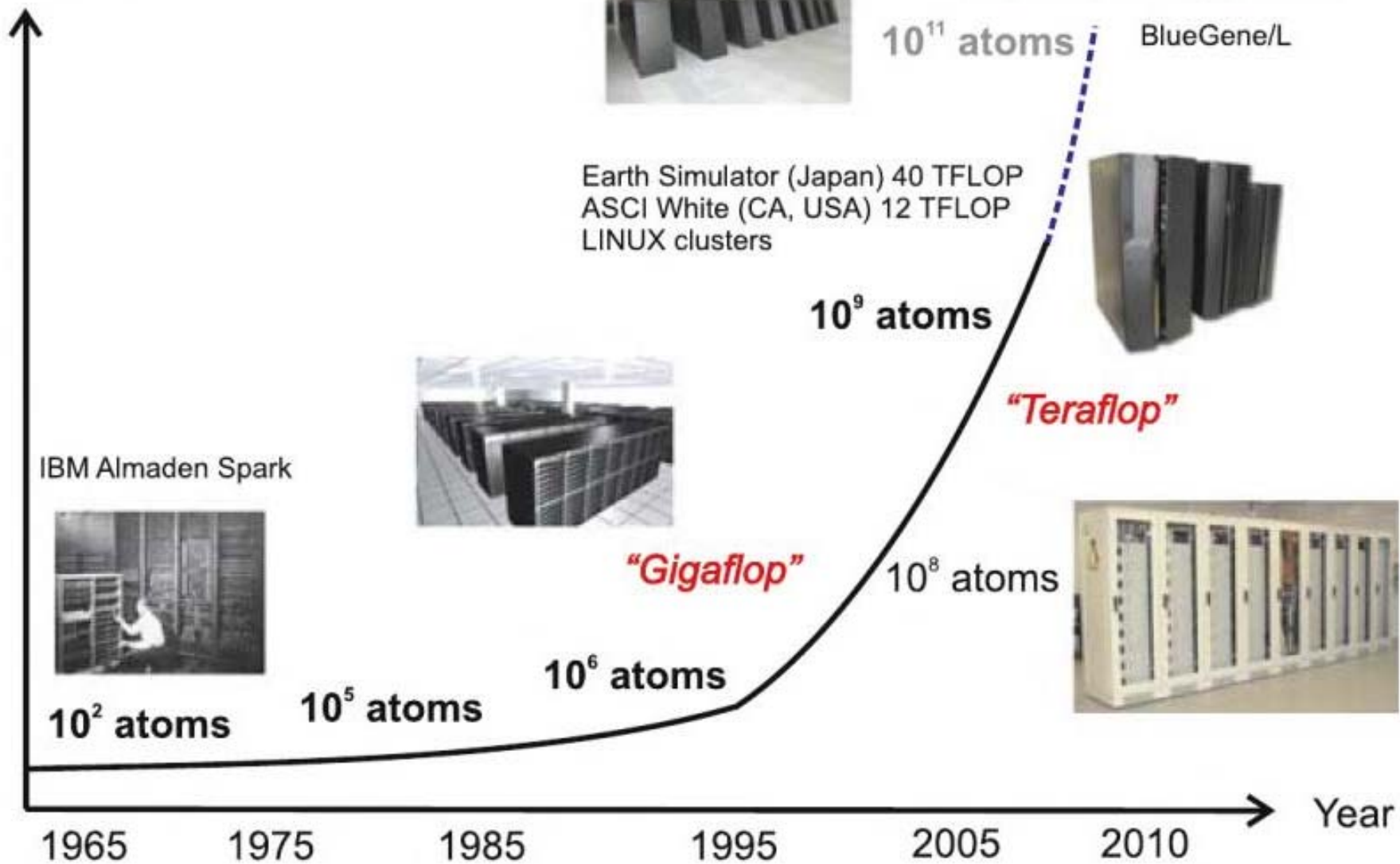
Multi-scale simulation paradigm



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2. Computing power: A perspective

Computing power



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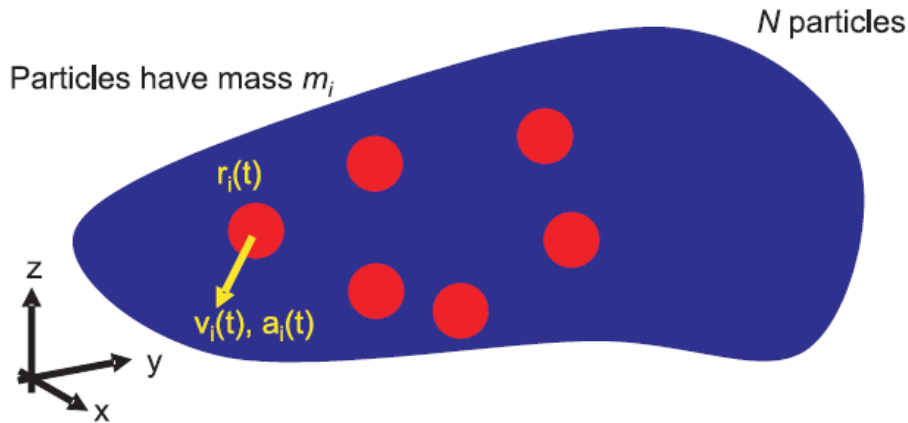
Historical development of computer simulation

- Began as tool to exploit computing machines developed during World War II
- MANIAC (1952) at Los Alamos used for computer simulations
- Metropolis, Rosenbluth, Teller (1953): Metropolis Monte Carlo method
- Alder and Wainwright (Livermore National Lab, 1956/1957): dynamics of hard spheres
- Vineyard (Brookhaven 1959-60): dynamics of radiation damage in copper
- Rahman (Argonne 1964): liquid argon
- Application to more complex fluids (e.g. water) in 1970s
- Car and Parrinello (1985 and following): *ab-initio* MD
- Since 1980s: Many applications, including:
 - Karplus, Goddard et al.: Applications to polymers/biopolymers, proteins since 1980s
 - Applications to fracture since mid 1990s to 2000
 - Other engineering applications (nanotechnology, e.g. CNTs, nanowires etc.) since mid 1990s-2000

3. How to calculate properties from atomistic simulation

A brief introduction to statistical mechanics

Molecular dynamics



Follow trajectories of atoms
(*classical mechanics,*
Newton's laws)

“Verlet central difference method”

$$r_i(t_0 + \Delta t) = -\underbrace{r_i(t_0 - \Delta t)}_{\text{Positions at } t_0 - \Delta t} + \underbrace{2r_i(t_0)}_{\text{Positions at } t_0} \Delta t + \underbrace{a_i(t_0)}_{\text{Accelerations at } t_0} (\Delta t)^2 + \dots$$

Positions
at $t_0 - \Delta t$

Positions
at t_0

Accelerations
at t_0

$$a_i = f_i / m$$

Property calculation: Introduction

Have:

$$\vec{x}(t), \dot{\vec{x}}(t), \ddot{\vec{x}}(t)$$

“microscopic information”

Want:

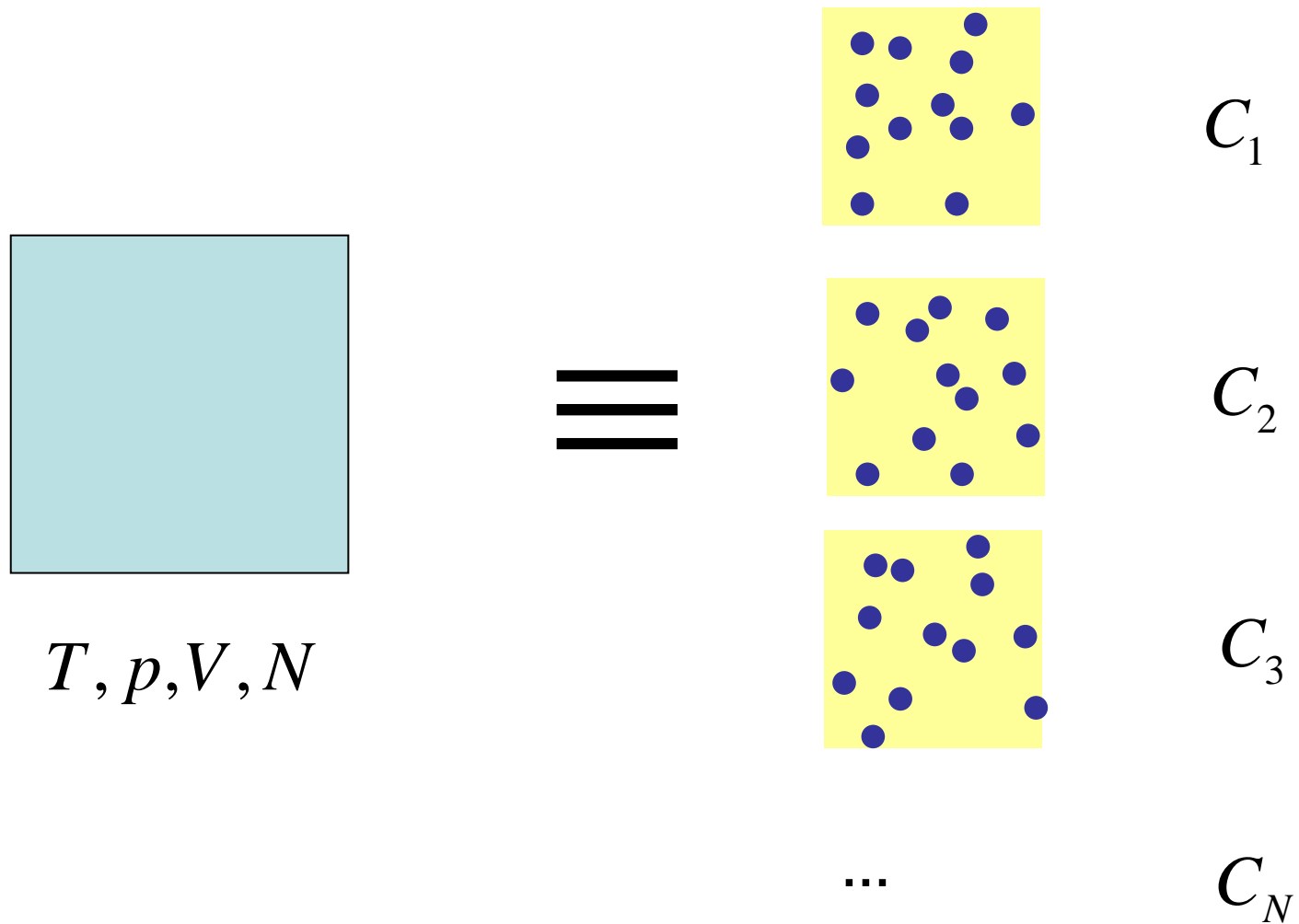
- Thermodynamical properties (temperature, pressure, stress, strain, thermal conductivity, ..)
- State (gas, liquid, solid)
- ...

(properties that can be measured in experiment!)

Goal: To develop a robust framework to calculate a range of “macroscale” properties from MD simulation studies (“microscale information”)

3.1 Thermodynamical ensembles: Micro and macro

Macroscopic vs. microscopic states



Same macroscopic state is represented by many different microscopic configurations C_i

Definition: Ensemble

- Large number of copies of a system with specific features
- Each copy represents a possible microscopic state a macroscopic system might be in under thermodynamical constraints ($T, p, V, N ..$)

Gibbs, 1878

Microscopic states

Microscopic states characterized by r, p

$$r = \{\vec{x}_i\}, p = \{m_i \dot{\vec{x}}_i\} \quad i = 1..N$$
$$\parallel$$
$$p_i$$

Microscopic states

Microscopic states characterized by r, p

$$r = \{\vec{x}_i\}, p = \{m_i \dot{\vec{x}}_i\} \quad i = 1..N$$
$$\parallel$$
$$p_i$$

Hamiltonian (sum of potential and kinetic energy = total energy)
expressed in terms of these variables

$$H(r, p) = U(r) + K(p)$$

$$U(r) = \sum_{i=1..N} \phi_i(r) \quad K(p) = \sum_{i=1..N} \frac{1}{2} \frac{p_i^2}{m_i} \leftarrow K_i = \frac{1}{2} m_i v_i^2$$

Ensembles

Result of thermodynamical constraints, e.g. temperature, pressure...

Microcanonical

NVE

Canonical

NVT

Isobaric-isothermal

NpT

Grand canonical

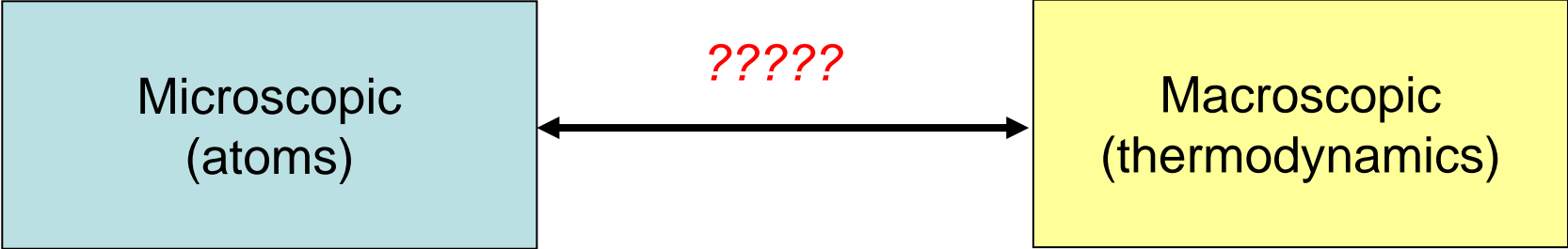
$TV\mu$

μ

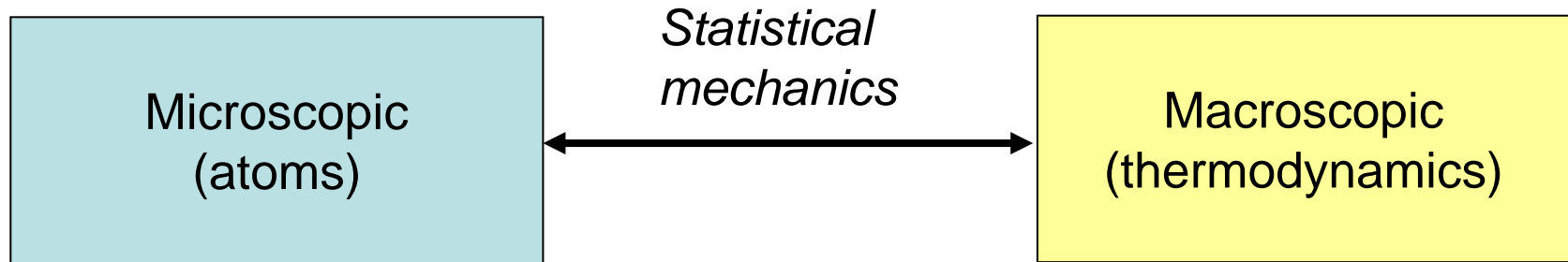
chemical potential (e.g. concentration)

3.2 How to calculate properties from atomistic simulation

Link between statistical mechanics and thermodynamics



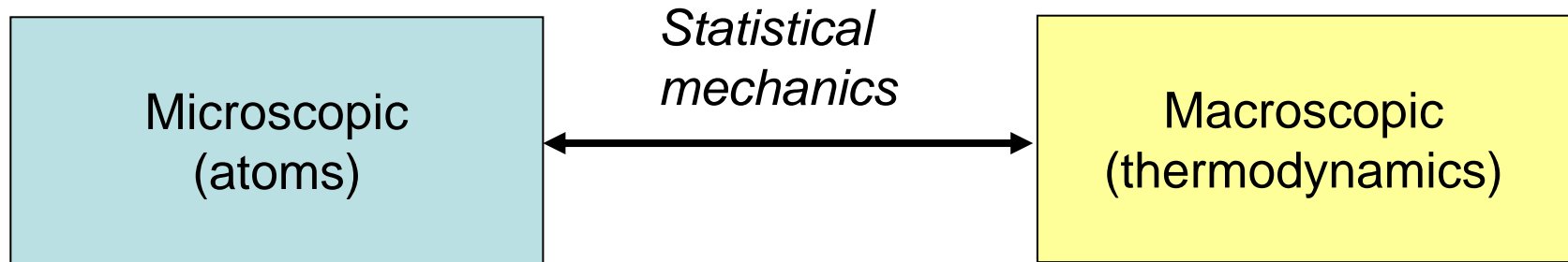
Link between statistical mechanics and thermodynamics



Macroscopic conditions (e.g. constant volume, temperature, number of particles...) translate to the microscopic system as boundary conditions (constraints)

Macroscopic system: defined by extensive variables, which are constant:
E.g. $(N, V, E) = NVE$ ensemble

Link between statistical mechanics and thermodynamics



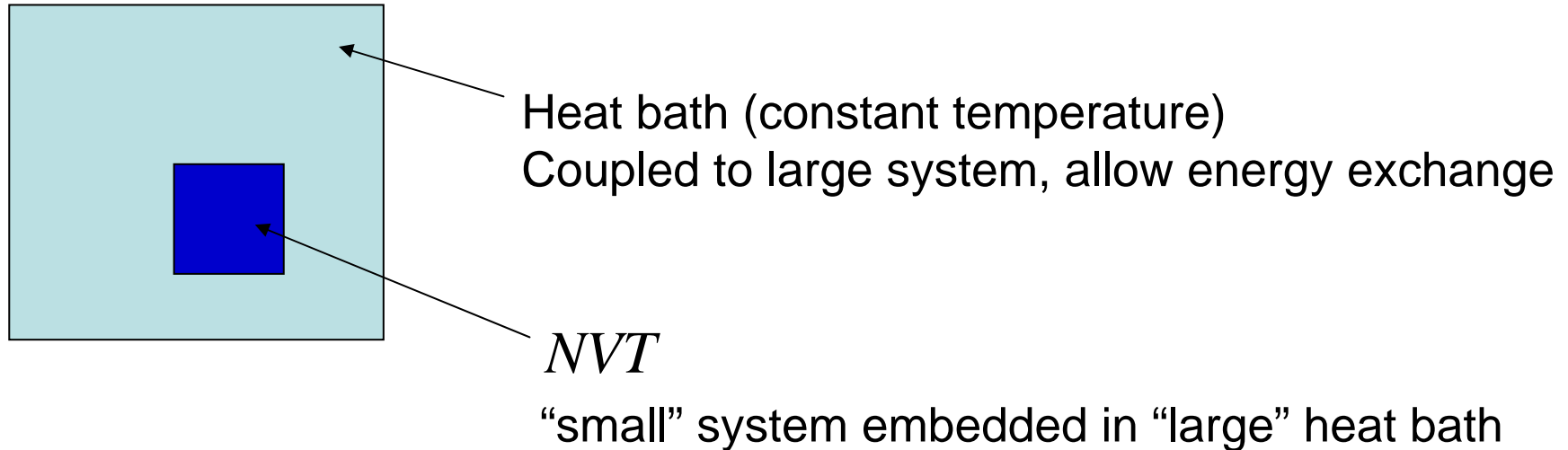
Macroscopic conditions (e.g. constant volume, temperature, number of particles...) translate to the microscopic system as boundary conditions (constraints)

Macroscopic system: defined by extensive variables, which are constant: E.g. $(N, V, E) = NVE$ ensemble

The behavior of the **microscopic system** is related to the macroscopic conditions. In other words, the distribution of microscopic states is related to the macroscopic conditions.

To **calculate macroscopic properties** (via statistical mechanics) from microscopic information we need to know the distribution of microscopic states (e.g. through a simulation)

Example: Physical realization of canonical ensemble (NVT)

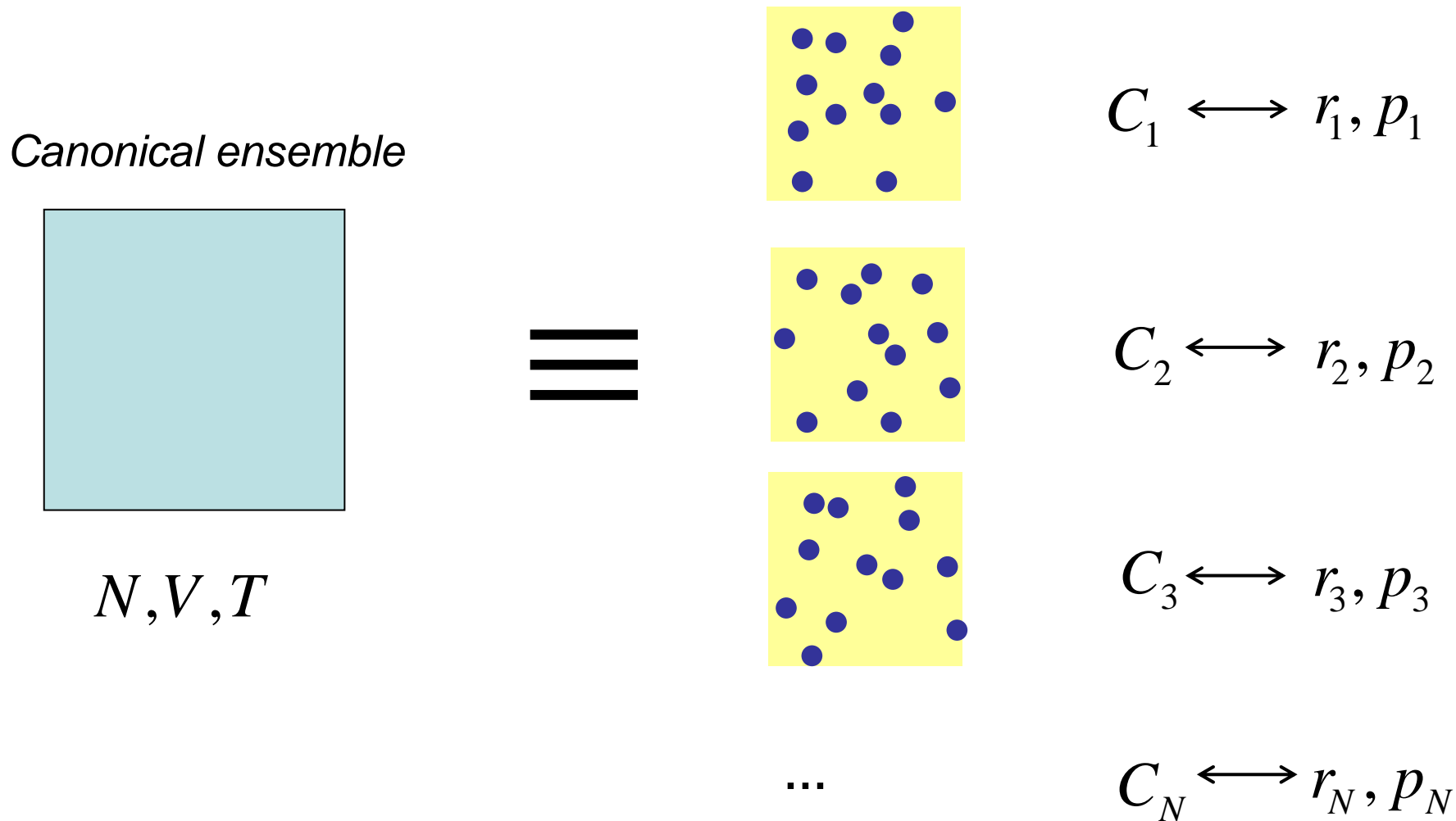


Constant number of particles = N

Constant volume = V

Constant temperature = T

Macroscopic vs. microscopic states



Same macroscopic state is represented by many different microscopic configurations

Important issue to remember...

- A few slides ago:

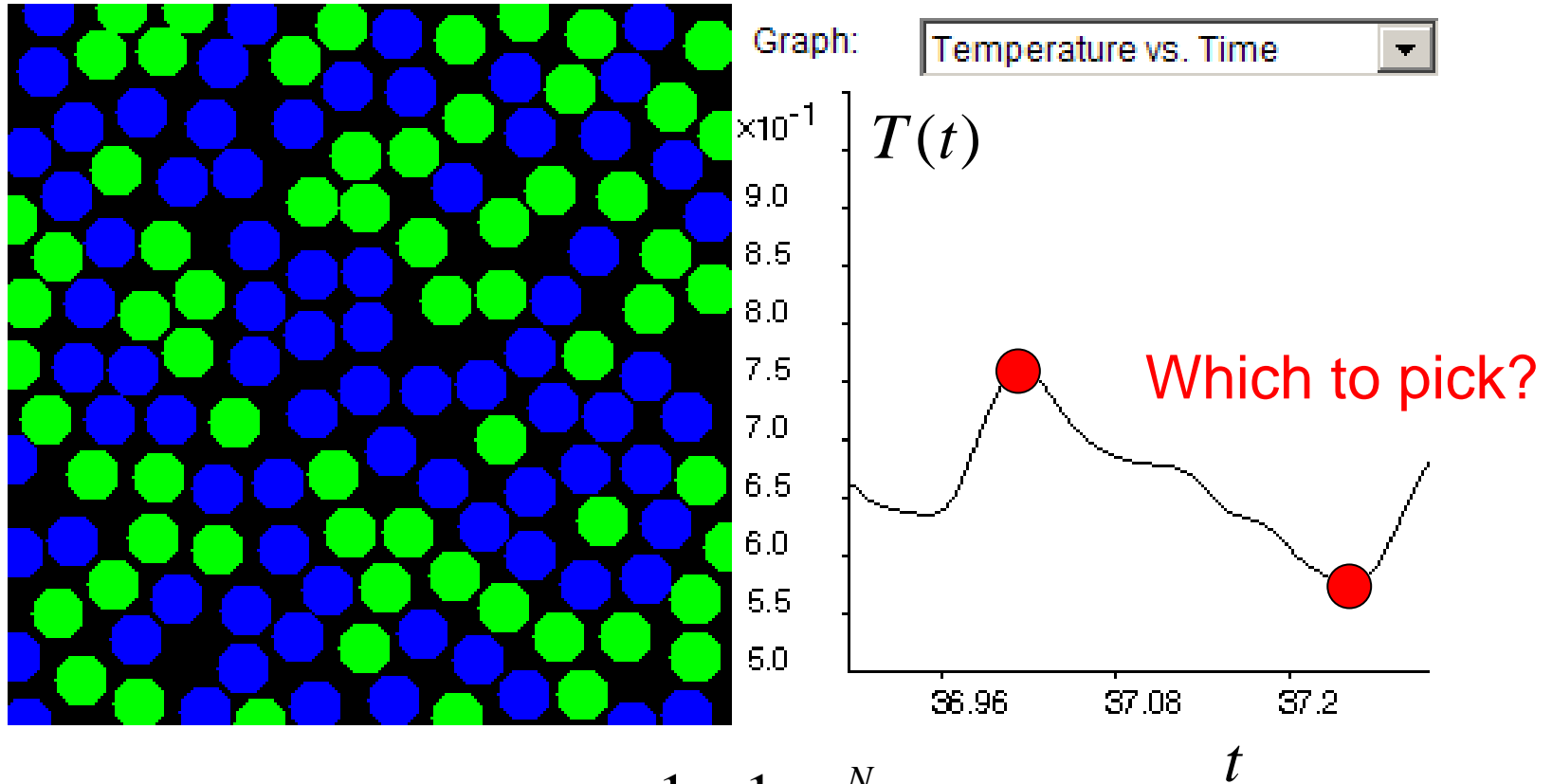
“To calculate macroscopic properties (via statistical mechanics) from microscopic information we need to know the distribution of microscopic states (e.g. through MD simulation)”

- **Therefore:**

We can not (“never”) take a single measurement from a single microscopic state to relate to macroscopic properties

Micro-macro relation

Courtesy of the Center for Polymer Studies at Boston University. Used with permission.



$$T(t) = \frac{1}{3} \frac{1}{Nk_B} \sum_{i=1}^N m_i \vec{v}_i^2(t)$$

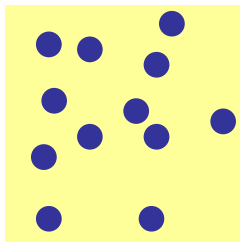
Specific (individual) microscopic states are insufficient to relate to macroscopic properties

Averaging over the ensemble

- Rather than taking single measurement, need to average over “all” microscopic states that represent the corresponding macroscopic condition
- This averaging needs to be done in a suitable fashion, that is, we need to **consider the specific distribution of microscopic states** (e.g. some microscopic states may be more likely than others)

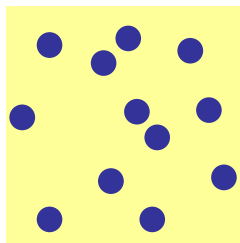
What about trying this....

Property A_1



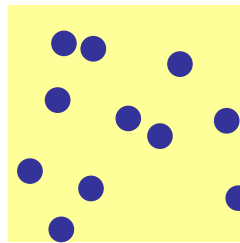
C_1
 r_1, p_1

Property A_2



C_2
 r_2, p_2

Property A_3



C_3
 r_3, p_3

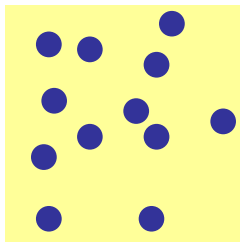
$$A_{\text{macro}} = \frac{1}{3} (A_1 + A_2 + A_3)$$

Averaging over the ensemble

- Rather than taking single measurement, need to average over “all” microscopic states that represent the corresponding macroscopic condition
- This averaging needs to be done in a suitable fashion, that is, we need to **consider the specific distribution of microscopic states** (e.g. some microscopic states may be more likely than others)

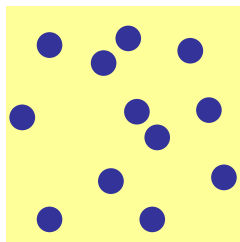
What about trying this....

Property A_1



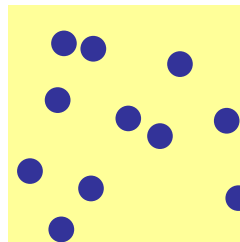
C_1

Property A_2



C_2

Property A_3



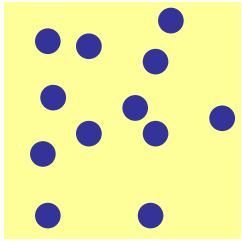
C_3

$$A_{\text{macro}} \neq \frac{1}{3} (A_1 + A_2 + A_3)$$

Generally, NO!

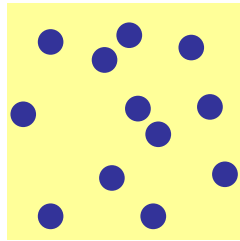
Averaging over the ensemble

Property A_1



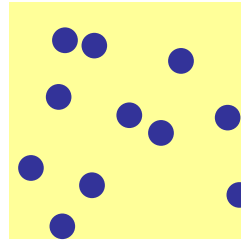
C_1

Property A_2



C_2

Property A_3



C_3

$$A_{\text{macro}} \neq \frac{1}{3} (A_1 + A_2 + A_3)$$

Instead, we must average with proper weights that represent the probability of a system in a particular microscopic state!

(I.e., not all microscopic states are equal)

$$A_{\text{macro}} = \rho_1 A_1 + \rho_2 A_2 + \rho_3 A_3 =$$

$$\rho_1(r_1, p_1) A_1(r_1, p_1) + \rho_2(r_2, p_2) A_2(r_2, p_2) + \rho_3(r_3, p_3) A_3(r_3, p_3)$$



Probability to find system in state C_1

How to relate microscopic states to macroscopic variables?

$A(r, p)$ Property due to specific microstate

$$\langle A \rangle = \int \int_{p, r} A(p, r) \rho(p, r) dr dp$$

- Ensemble average, obtained by integral over all microscopic states
- Proper weight $\rho(p, r)$ - depends on ensemble

How to relate microscopic states to macroscopic variables?

$A(r, p)$ Property due to specific microstate

To measure an observable quantity from MD simulation we must express this observable as a function of the positions and linear momenta of the particles in the system, that is, r, p

Recall, microscopic states characterized by r, p

$$r = \{\vec{x}_i\}, p = \{m_i \dot{\vec{x}}_i\} \quad i = 1..N$$
$$\parallel$$
$$p_i$$

How to relate microscopic states to macroscopic variables?

$$\langle A \rangle = \int \int_{p, r} A(p, r) \rho(p, r) dr dp$$

Probability density distribution

$$\rho(p, r) = \frac{1}{Q} \exp\left[-\frac{H(p, r)}{k_B T}\right]$$

Probability to find system in state (p, r)

Boltzmann constant

$$k_B = 1.3806503 \times 10^{-23} \text{ m}^2 \text{ kg s}^{-2} \text{ K}^{-1}$$

Partition function

$$Q = \int \int_{p, r} \exp\left[-\frac{H(p, r)}{k_B T}\right] dr dp$$

Illustration/example: phase space

*6N-dimensional
phase space*

Image removed due to copyright restrictions. See the second image at <http://www.ace.gatech.edu/experiments2/2413/lorenz/fall02/>.

$$\begin{array}{c} r, p \\ \downarrow \\ \rho(p, r) \end{array}$$

Definition of temperature

Classical (mechanics) many-body system:

Average kinetic energy per degree of freedom is related to temperature via Boltzmann constant.

$$\left\langle \frac{1}{2} m \vec{v}_i^2 \right\rangle = \frac{1}{N_f} \sum_{i=1..N_f} \left(\frac{1}{2} m \vec{v}_i^2 \right) = \frac{1}{2} k_B T$$

DOF

$$N_f = 3N$$

particles (each 3 DOF for velocities)

Based on equipartition theorem (energy distributed equally over all DOFs)

Definition of temperature

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DOF

$$N_f = 3N$$

$= p_i$

$$T(p) = \frac{1}{3} \frac{1}{N k_B} \sum_{i=1}^N \frac{m_i^2 \vec{v}_i^2}{m_i} = A(p)$$

Temperature

How to calculate temperature

$$\langle T \rangle = \int_p \int_r \frac{1}{3} \frac{1}{Nk_B} \sum_{i=1}^N \frac{m_i^2 \vec{v}_i^2}{m_i} \rho(p, r) dr dp$$

↑
???

How to solve...

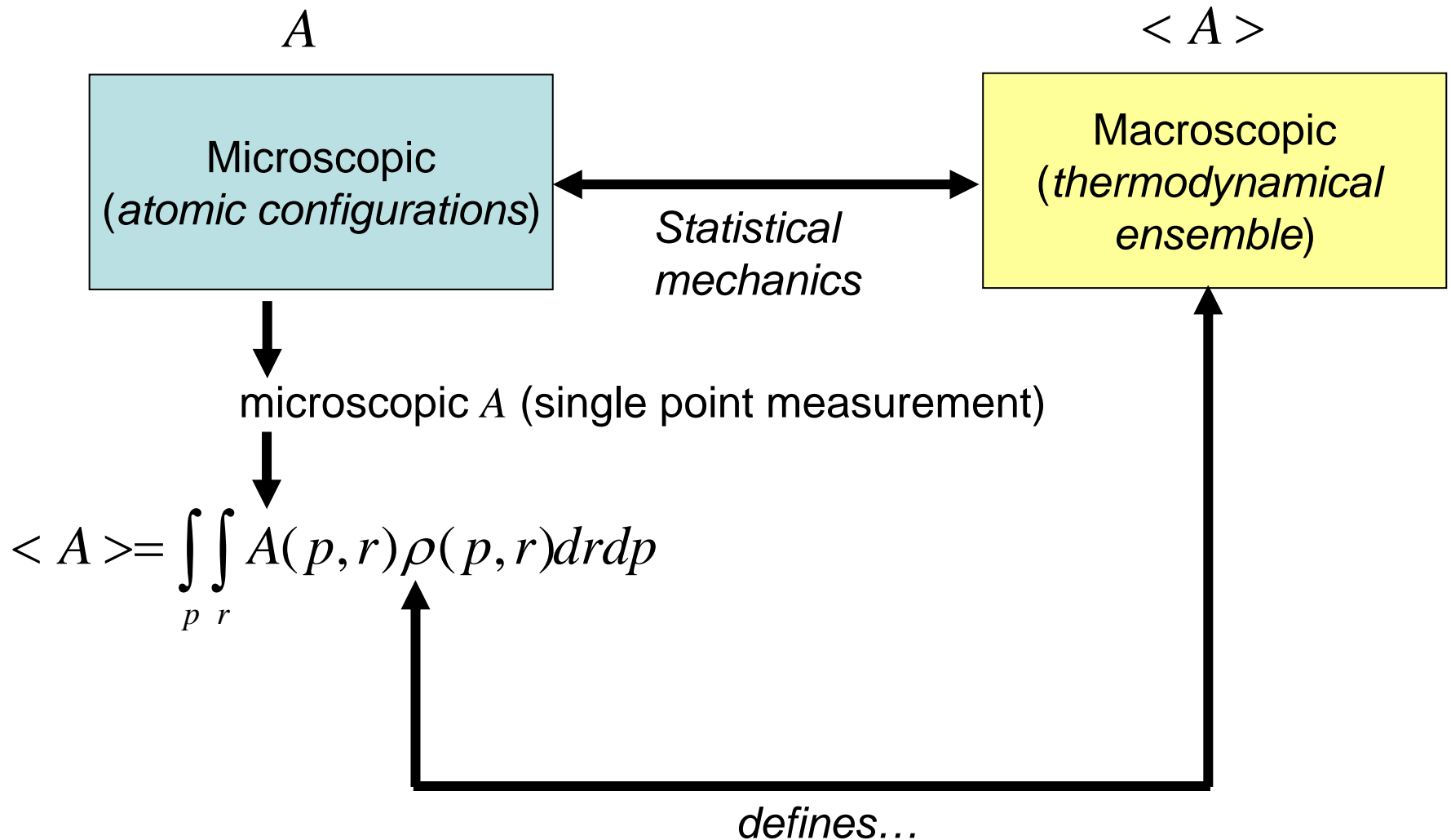
$$\langle A \rangle = \int \int_{p \ r} A(p, r) \rho(p, r) dr dp$$

Virtually impossible to carry out analytically

Must know all possible microscopic configurations corresponding to a macroscopic ensemble, then calculate ρ

Therefore: Require numerical simulation (the only feasible approach...)

Summary: How macro-micro relation works



3.3 How to solve the equations

Approaches in solving this problem

- **Method of choice: *Numerical simulation***
- Two major approaches:
 1. Using **molecular dynamics (MD)**: Generate microscopic information through dynamical evolution of microscopic system (*i.e.*, simulate the “real behavior” as we would obtain in lab experiment)
 2. Using a numerical scheme/algorithm to randomly generate microscopic states, which, through proper averaging, can be used to compute macroscopic properties. Methods referred to as “**Monte Carlo**”

Monte Carlo (MC) scheme

- Concept: Find simpler way to solve the integral

$$\langle A \rangle = \int \int_{p \ r} A(p, r) \rho(p, r) dr dp$$

- Use idea of “random walk” to step through relevant microscopic states and thereby create proper weighting (visit states with higher probability density more often)

=ensemble (statistical) average

MC algorithm result

Final result of MC algorithm:

*Algorithm that leads to proper
Distribution of microscopic states...*

$$\langle A \rangle = \int \int_{p \ r} A(p, r) \rho(p, r) dr dp$$



*Ensemble
(statistical)
average*

$$\langle A \rangle = \frac{1}{N_A} \sum_i A_i$$

*Carry out algorithm
for N_A steps
Average results
..done!*

3.4 Ergodic hypothesis

Ergodicity

- MC method is based on directly computing the ensemble average

Define a series of microscopic states that reflect the appropriate ensemble average; weights intrinsically captured since states more likely are visited more frequently and vice versa

- **Ergodicity:** The ensemble average is equal to the time-average during the dynamical evolution of a system under proper thermodynamical conditions.

In other words, the set of microscopic states generated by solving the equations of motion in MD “automatically” generates the proper distribution/weights of the microscopic states

This is called the Ergodic hypothesis:

$$\langle A \rangle_{Ens} = \langle A \rangle_{Time}$$

Ergodic hypothesis

- Ergodic hypothesis:

Ensemble (statistical) average = time average

- All microstates are sampled with appropriate probability density over long time scales

$$\underbrace{\frac{1}{N_A} \sum_{i=1..N_A} A(i)}_{\text{MC}} = \langle A \rangle_{\text{Ens}} = \langle A \rangle_{\text{Time}} = \underbrace{\frac{1}{N_t} \sum_{i=1..N_t} A(i)}_{\text{MD}}$$

Ergodic hypothesis

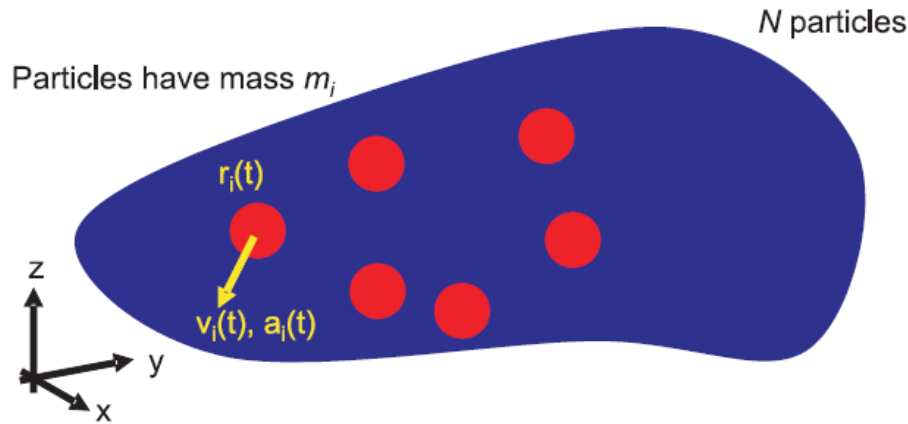
- Ergodic hypothesis:

Ensemble (statistical) average = time average

- All microstates are sampled with appropriate probability density over long time scales

$$\underbrace{\frac{1}{N_A} \sum_{i=1..N_A} \left(\frac{1}{3} \frac{1}{Nk_B} \sum_{i=1}^N m_i \vec{v}_i^2 \right)}_{\text{MC}} = \langle A \rangle_{\text{Ens}} = \langle A \rangle_{\text{Time}} = \underbrace{\frac{1}{N_t} \sum_{i=1..N_t} \left(\frac{1}{3} \frac{1}{Nk_B} \sum_{i=1}^N m_i \vec{v}_i^2 \right)}_{\text{MD}}$$

Importance for MD algorithm



Follow trajectories of atoms
(*classical mechanics,*
Newton's laws)

“Verlet central difference method”

$$r_i(t_0 + \Delta t) = \underbrace{-r_i(t_0 - \Delta t)}_{\text{Positions at } t_0 - \Delta t} + \underbrace{2r_i(t_0)}_{\text{Positions at } t_0} \Delta t + \underbrace{a_i(t_0)}_{\text{Accelerations at } t_0} (\Delta t)^2 + \dots \quad a_i = f_i / m$$

It's sufficient to simply average over all MD steps...

$$\langle A \rangle_{Time} = \frac{1}{N_t} \sum_{i=1..N_t} A(i)$$

Molecular dynamics

- During integration of equations of motion – must impose thermodynamical constraints
- For example, *Verlet central difference method* leads to a microcanonical ensemble (*NVE*)
- Other integration methods exist to generate *NVT*, *NpT* ensembles etc.

$$r_i(t_0 + \Delta t) = \underbrace{-r_i(t_0 - \Delta t)}_{\text{Positions at } t_0 - \Delta t} + \underbrace{2r_i(t_0)\Delta t}_{\text{Positions at } t_0} + \underbrace{a_i(t_0)(\Delta t)^2}_{\text{Accelerations at } t_0} + \dots$$

$$a_i = f_i / m$$

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