From nano to macro: Introduction to atomistic modeling techniques
IAP 2007

Introduction to classical molecular dynamics (cont'd)

Mechanics of Ductile Materials

Lecture 3

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Outline

1. **Introduction to Mechanics of Materials**
   Basic concepts of mechanics, stress and strain, deformation, strength and fracture
   Monday Jan 8, 09-10:30am
2. **Introduction to Classical Molecular Dynamics**
   Introduction into the molecular dynamics simulation; numerical techniques
   Tuesday Jan 9, 09-10:30am
3. **Mechanics of Ductile Materials**
   Dislocations; crystal structures; deformation of metals
   Tuesday Jan 16, 09-10:30am
4. **Dynamic Fracture of Brittle Materials**
   Nonlinear elasticity in dynamic fracture, geometric confinement, interfaces
   Wednesday Jan 17, 09-10:30am
5. **The Cauchy-Born rule**
   Calculation of elastic properties of atomic lattices
   Friday Jan 19, 09-10:30am
6. **Mechanics of biological materials**
   Monday Jan. 22, 09-10:30am
7. **Introduction to The Problem Set**
   Atomistic modeling of fracture of a nanocrystal of copper.
   Wednesday Jan 22, 09-10:30am
8. **Size Effects in Deformation of Materials**
   Size effects in deformation of materials: Is smaller stronger?
   Friday Jan 26, 09-10:30am

Historic MD references

- Alder, B. J. and Wainwright, T. E. *J. Chem. Phys.* **27**, 1208 (1957)
- Alder, B. J. and Wainwright, T. E. *J. Chem. Phys.* **31**, 459 (1959)

- Rahman, A. *Phys. Rev.* **A136**, 405 (1964)

- Stillinger, F. H. and Rahman, A. *J. Chem. Phys.* **60**, 1545 (1974)

- McCammon, J. A., Gelin, B. R., and Karplus, M. *Nature (Lond.)* **267**, 585 (1977)

Outline and content (Lecture 3)

- **Topic:** Basic molecular dynamics (MD), interatomic forces, property calculation
- **Examples:** Movie of 1,000,000,000 atom simulation
  Simple Java applets
- **Material covered:** Review, computing strategies, radial distribution function, diffusion, virial stress
- **Important lesson:** How to link microscopic atomistic processes and properties with macroscopic observables; first simple model for interatomic potential
- **Historical perspective:** Early MD simulations: Thermodynamical properties of water or noble gases (1960s)

A simulation with 1,000,000,000 particles

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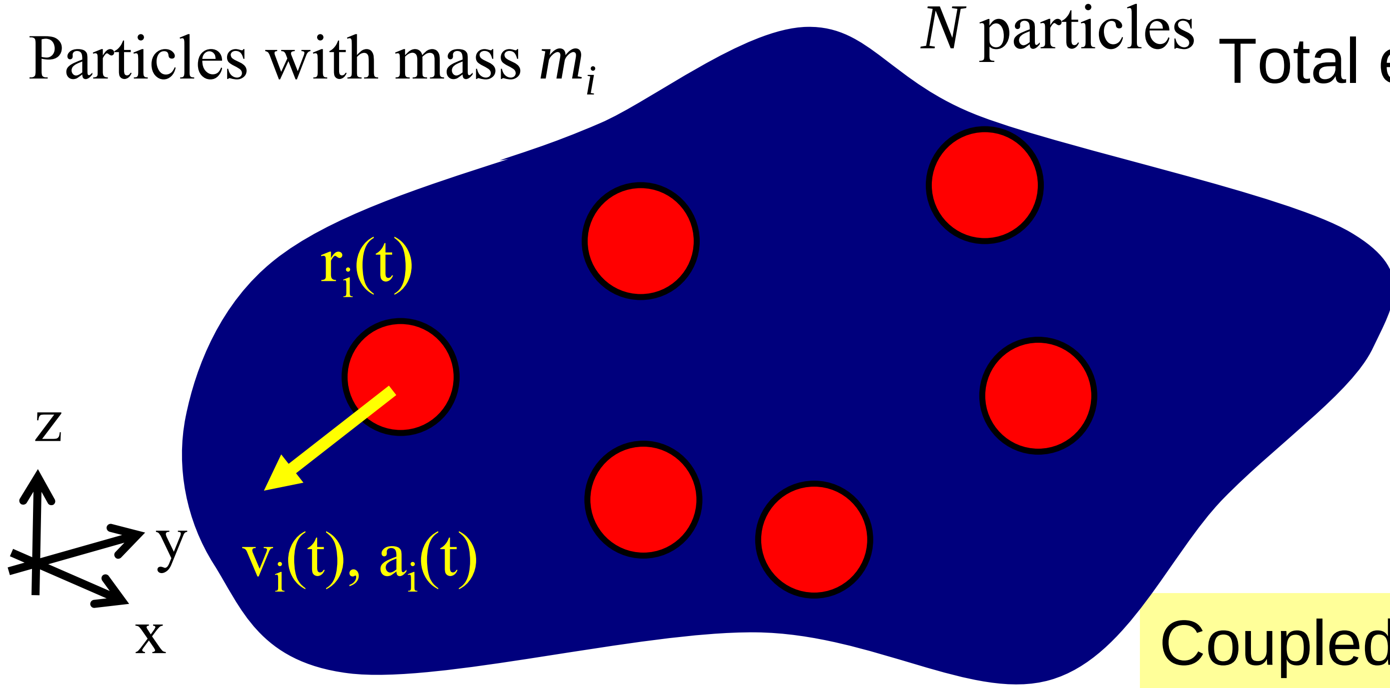
(F. Abraham, *et al*.)

Molecular dynamics

Particles with mass m_i

N particles



Total energy of system

$$E = K + U$$

$$K = \frac{1}{2} m \sum_{j=1}^{N} v_j^2$$

$$U = U(r_j)$$

Coupled system N-body problem, no exact solution for *N*>2

$$m \frac{d^2 r_j}{dt^2} = -\nabla_{r_j} U(r_j) \qquad j = 1..N$$

System of coupled 2[nd] order nonlinear differential equations

Solve by discretizing in time (spatial discretization given by "atom size")

Solving the equations

$$r_i(t_0) \rightarrow r_i(t_0+\Delta t) \rightarrow r_i(t_0+2\Delta t) \rightarrow r_i(t_0+3\Delta t) \rightarrow \ldots \rightarrow r_i(t_0+n\Delta t)$$

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

Positions at t_0-Δt

Velocities at t_0

Accelerations at t_0

"Verlet central difference method"

How to obtain accelerations?

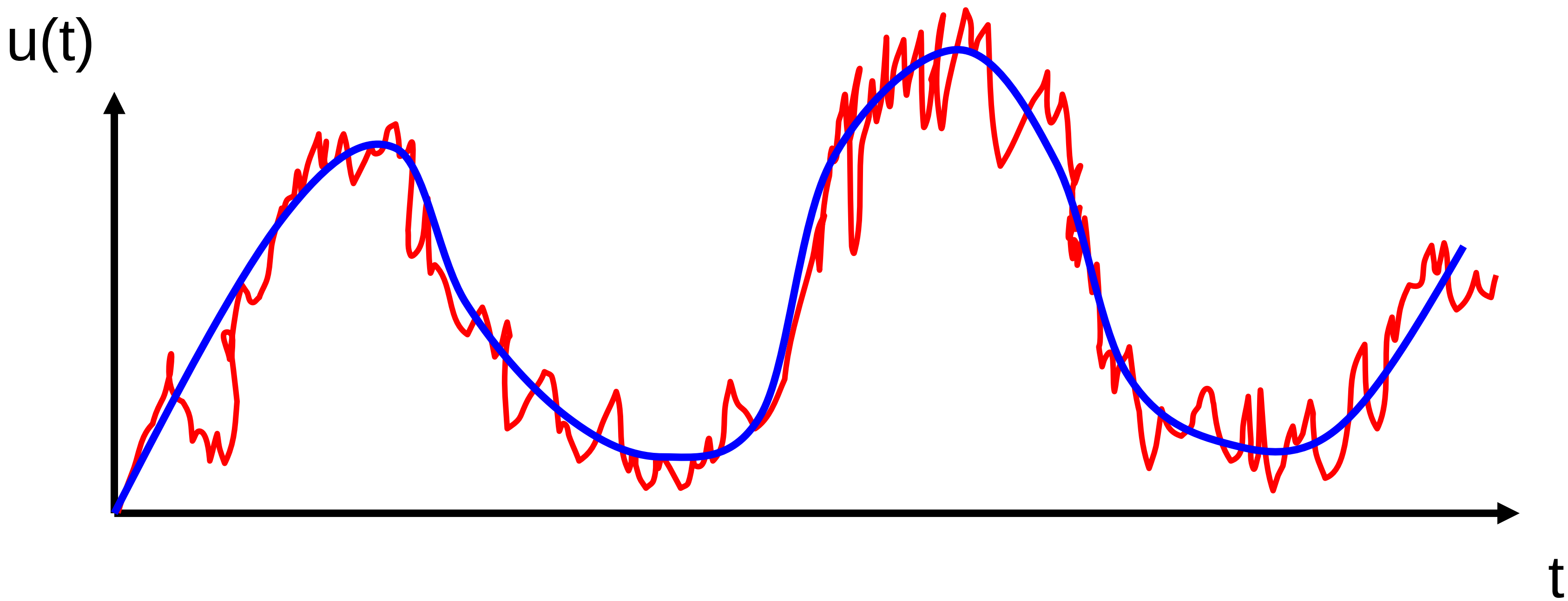
$$f_i = m a_i$$

$$a_i = f_i / m$$

Need forces on atoms!

Time-discretization

- Time step Δt needs to be small enough to model the vibrations of atomic bonds correctly
- Vibration frequencies may be extremely high, in particular for light atoms
- Thus: Time step on the order of 0.1..5 fs (10^{-15} seconds)
- Need 1,000,000 integration steps to calculate trajectory over 1 nanosecond: Significant computational burden…



Periodic boundary conditions

- Sometimes, have **periodic boundary conditions**; this allows studying bulk properties (no free surfaces) with small number of particles *(here: N=3!) – all particles are "connected"*
  - Original cell surrounded by 26 image cells; image particles move in exactly the same way as original particles (8 in 2D)

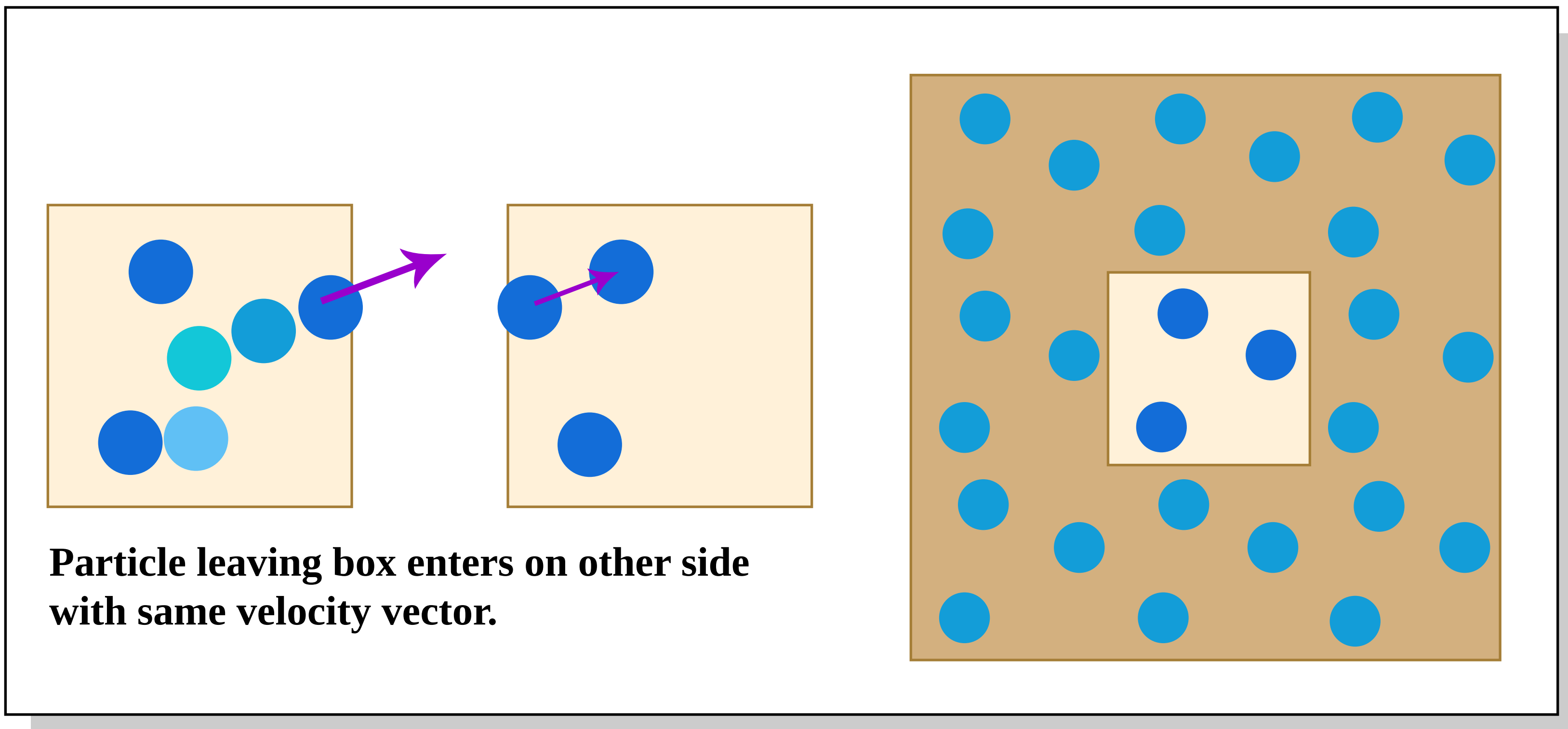


Figure by MIT OCW. After Buehler.

Numerical implementation of MD

How are forces calculated?

- Forces required to obtain accelerations to integrate EOM…
- Forces are calculated based on the distance between atoms; while considering some interatomic potential surface
- In principle, all atoms in the system interact with all atoms: Need nested loop

$$F = m\frac{d^2 r_j}{dt^2} = \underbrace{-\nabla_{r_j} U(r_j)}_{} \qquad j = 1..N$$

Force: Partial derivative of potential energy with respect to atomic coordinates

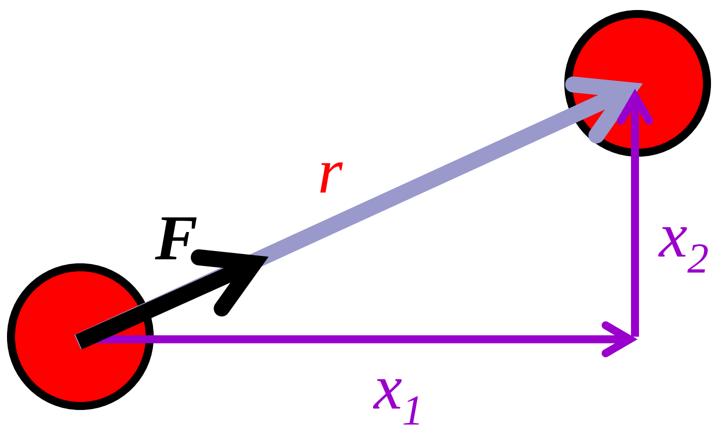
How are forces calculated?

Force magnitude: Derivative of potential energy with respect to atomic distance

$$F = -\frac{\mathrm{d}\,\phi(r)}{\mathrm{d}\,r}$$

To obtain force vector F_i, take projections into the three axial directions

$$F_i = F\,\frac{x_i}{r}$$



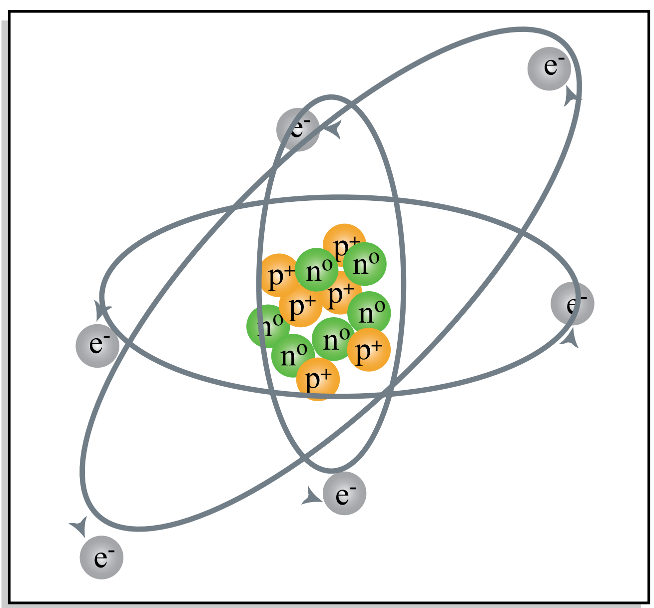
Assume pair-wise interaction between atoms

Atomic scale

- Atoms are composed of electrons, protons, and neutrons. Electron and protons are negative and positive charges of the same magnitude, 1.6 × 10-19 Coulombs
- Chemical bonds between atoms by interactions of the electrons of different atoms

(see QM part
later in IM/S!)

"Point" representation



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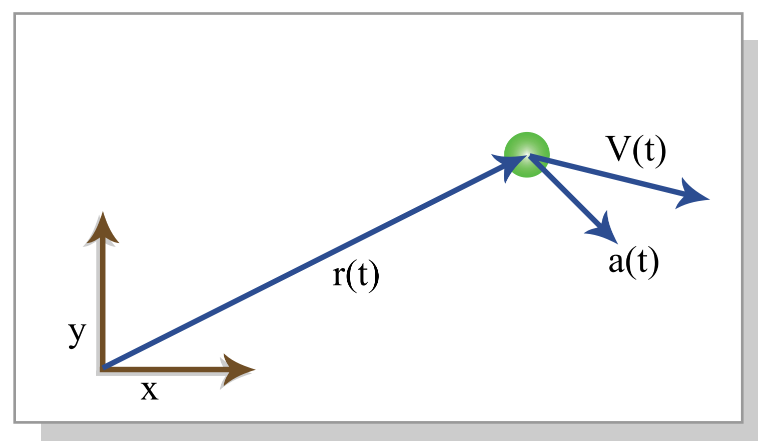

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Atomic interactions

- **Primary bonds ("strong")**
  - Ionic,
  - Covalent,
  - Metallic (high melting point, 1000-5000K)

- **Secondary bonds ("weak")**
  - Van der Waals,
  - Hydrogen bonds
    (melting point 100-500K)

- Ionic: Non-directional
- Covalent: Directional (angles, torsions)
- Metallic: Non-directional

Models for atomic interactions

- Atom-atom interactions are necessary to compute the forces and accelerations at each MD time integration step: Update to new positions!

- Usually define interatomic potentials, that describe the energy of a set of atoms as a function of their coordinates:

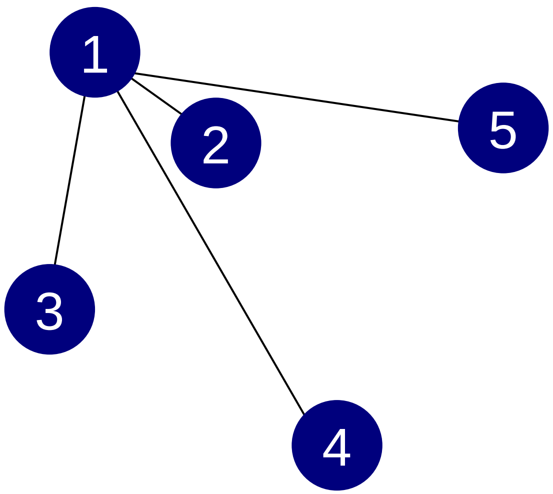
$$U_{total} = U_{total}(r_i)$$

- Simple approximation: Total energy is sum over the energy of all pairs of atoms in the system

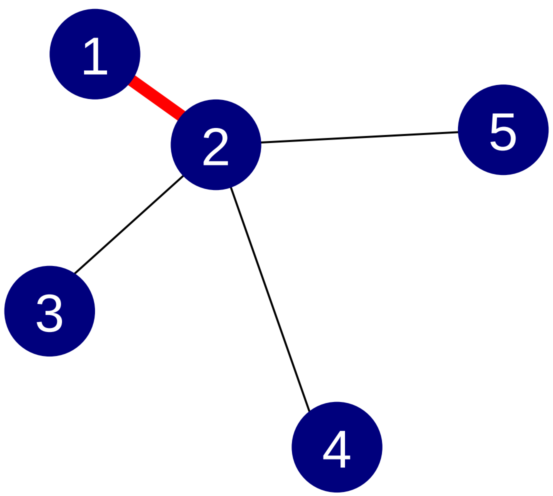
$$U_{total} = \frac{1}{2} \sum_{i \neq j} U(r_{ij})$$

Pair interaction approximation

$$U_{total} = \frac{1}{2}\sum_{i \neq j} U(r_{ij})$$



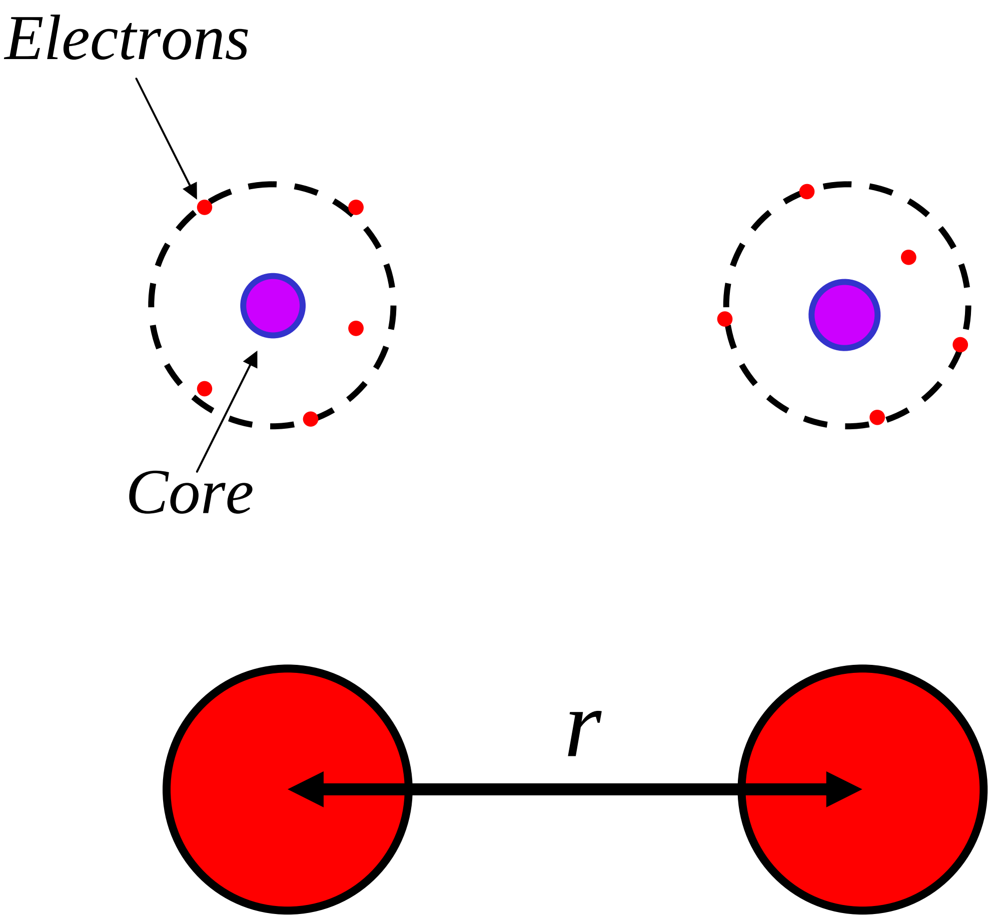
All pair interactions of atom 1 with neighboring atoms 2..5

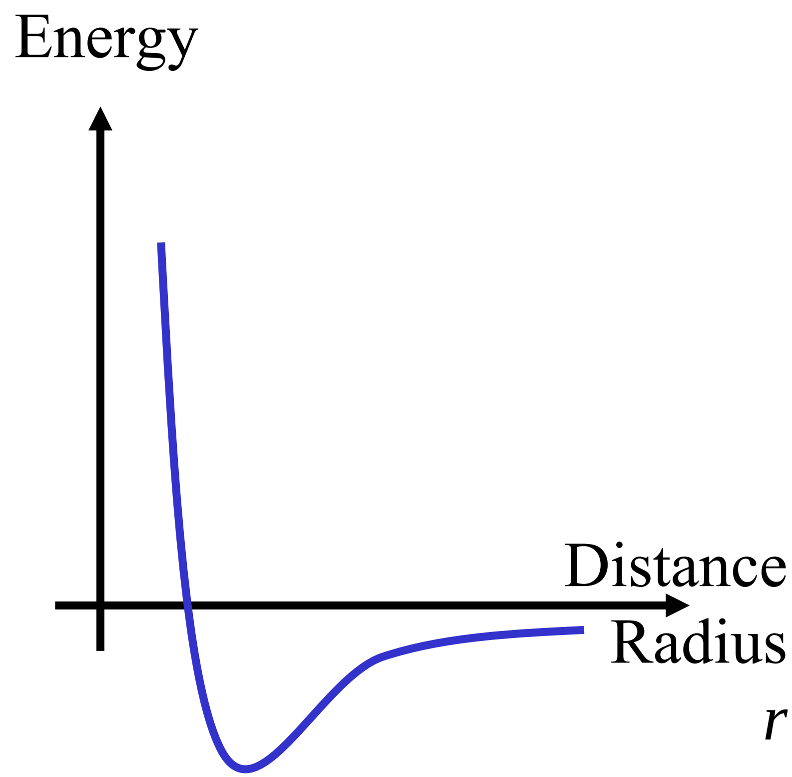


All pair interactions of atom 2 with neighboring atoms 1, 3..5

Double count bond 1-2 therefore factor $\frac{1}{2}$

From electrons to atoms





Governed by laws of quantum mechanics: Numerical solution by Density Functional Theory (DFT), for example

Repulsion versus attraction

- Repulsion: Overlap of electrons in same orbitals; according to Pauli exclusion principle this leads to high energy structures
  Model: *Exponential term*

- Attraction: When chemical bond is formed, structure (bonded atoms) are in local energy minimum; breaking the atomic bond costs energy – results in attractive force

- Sum of repulsive and attractive term results in the typical potential energy shape:

$$U = U_{rep} + U_{attr}$$

Lennard-Jones potential

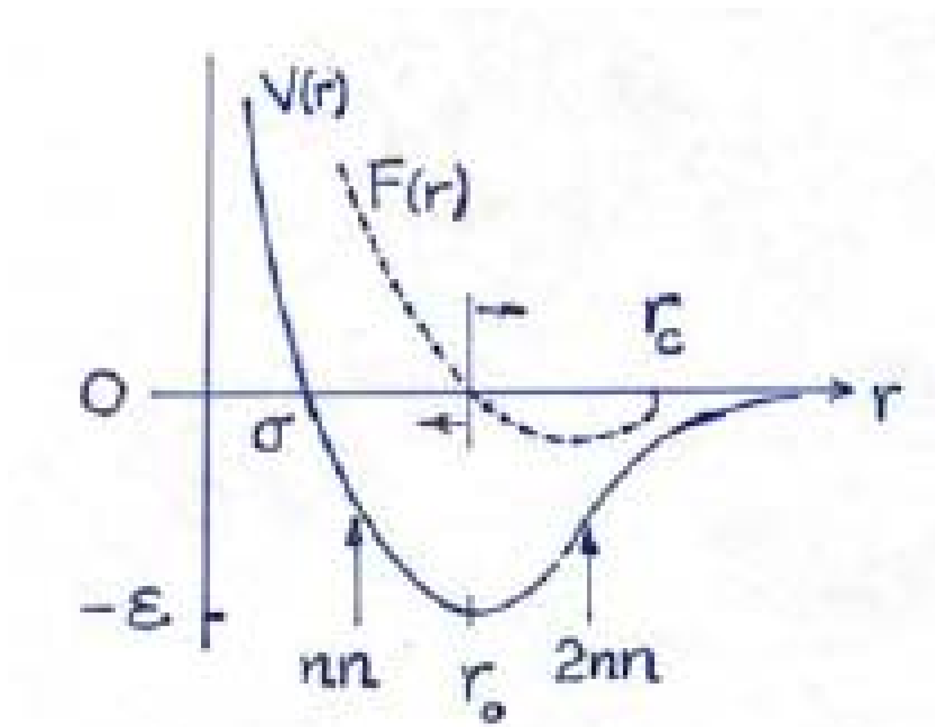
Attractive

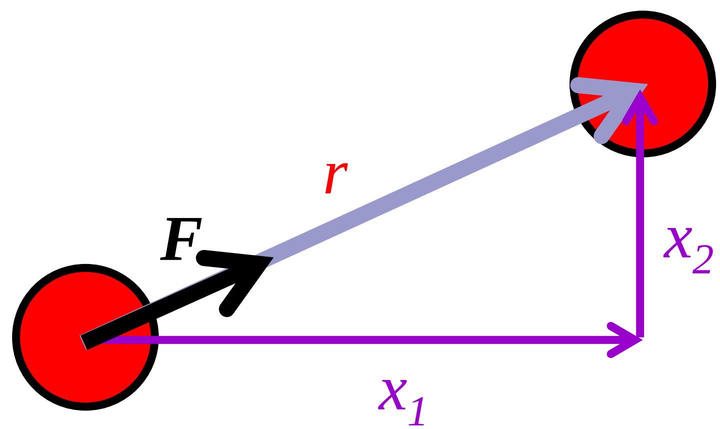
$$\phi(r) = 4\varepsilon\left(\left[\frac{\sigma}{r}\right]^{12} - \left[\frac{\sigma}{r}\right]^{6}\right)$$

Repulsive

$$F = -\frac{\mathrm{d}\,\phi(r)}{\mathrm{d}\,r}$$

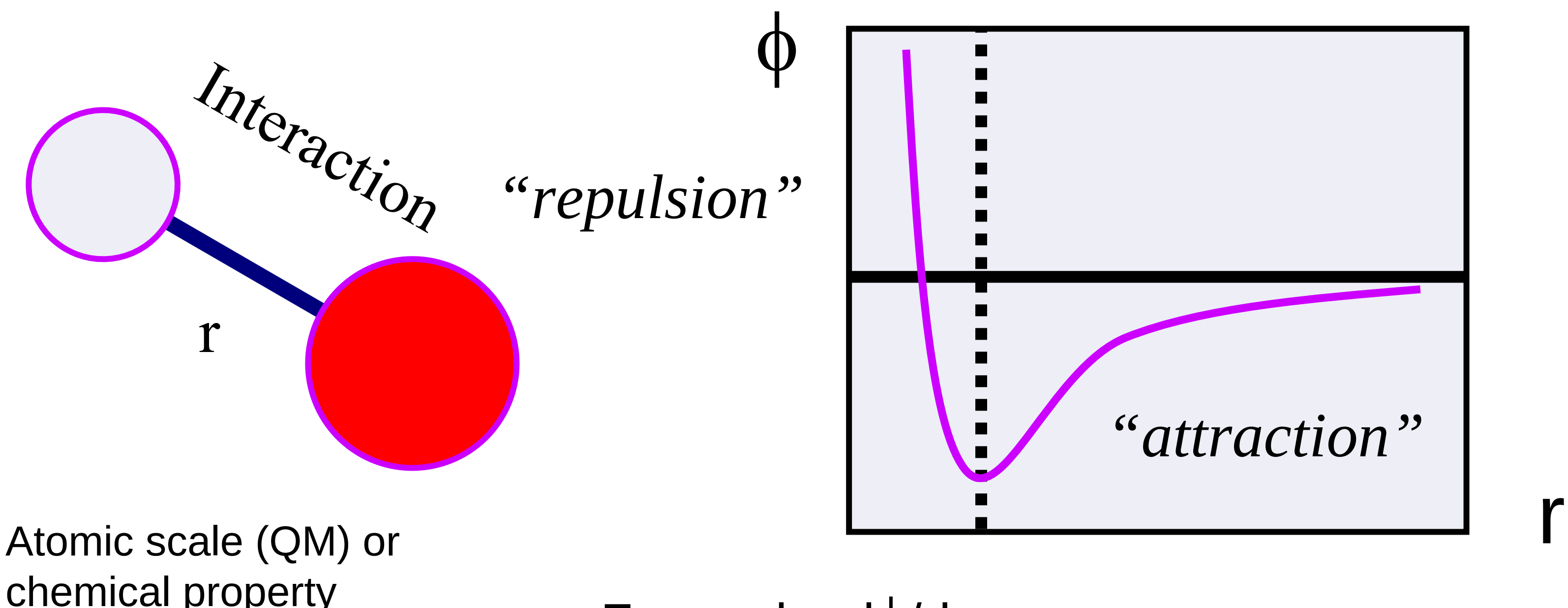
$$F_i = F\,\frac{x_i}{r}$$





The interatomic potential

- The fundamental input into molecular simulations, in addition to structural information (position of atoms, type of atoms and their velocities/accelerations) is provided by definition of the interaction potential (equiv. terms often used by chemists is "force field")
- MD is very general due to its formulation, but hard to find a "good" potential (extensive debate still ongoing, choice depends very strongly on the application)
- Popular: Semi-empirical or empirical (fit of carefully chosen mathematical functions to reproduce the potential energy surface…)



Forces by $d\phi/dr$

Lennard-Jones potential: Properties

$$\phi(r) = 4\varepsilon\left(\left[\frac{\sigma}{r}\right]^{12} - \left[\frac{\sigma}{r}\right]^{6}\right)$$

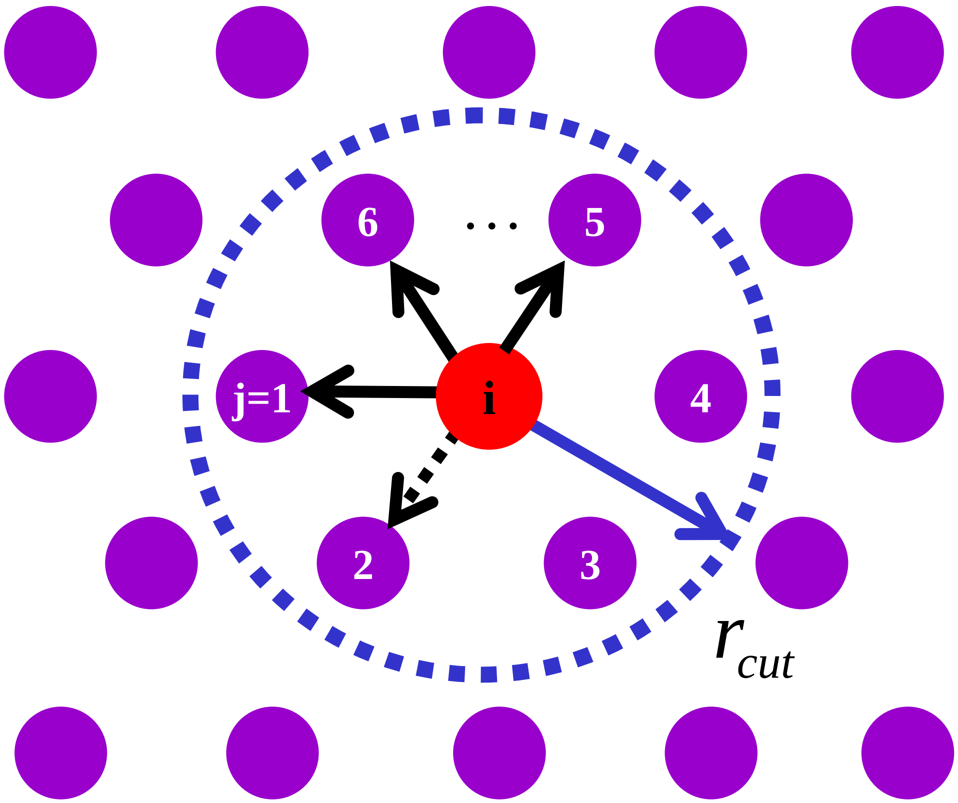
ε: Well depth (energy per bond)

σ: Potential vanishes

Equilibrium distance between atoms r_0 and maximum force

$$\sigma\sqrt[6]{2} = r_0 \qquad F_{\max,LJ} = \frac{2.394\cdot\varepsilon}{\sigma}$$

Pair potentials



$$\phi_i = \sum_{j=1..N_{neigh}} \varphi(r_{ij})$$

Lennard-Jones 12:6

$$\varphi(r_{ij}) = 4\varepsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right]$$

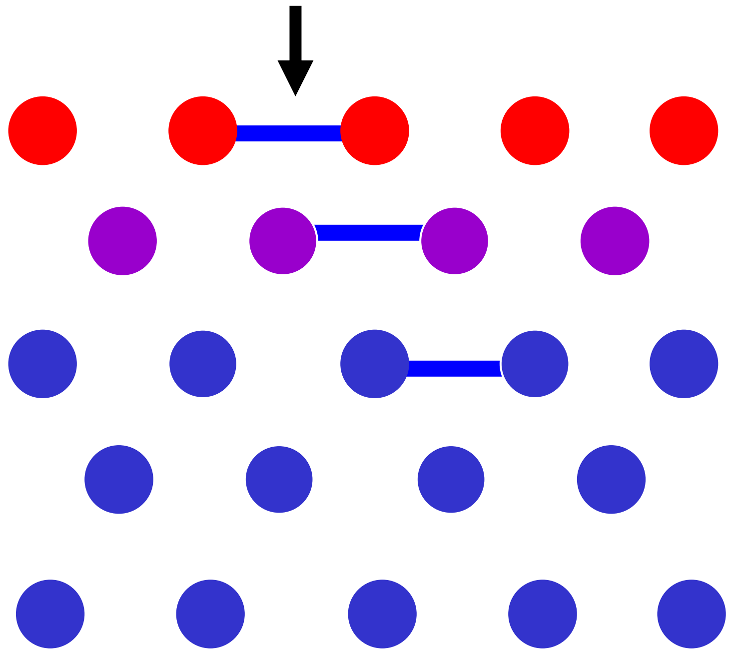
Morse

$$\varphi(r_{ij}) = D\{1 - \exp[-\beta(r_{ij} - r_0)]\}^2$$

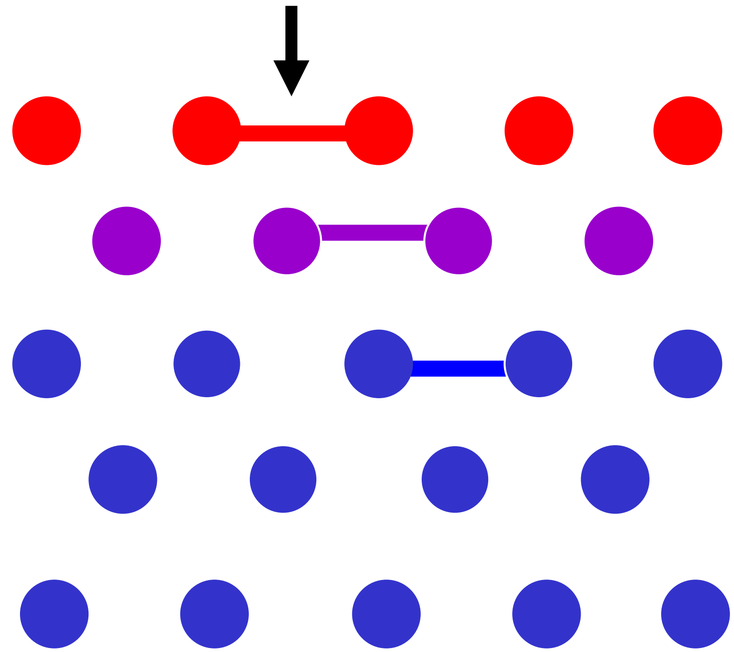
Reasonable model for noble gas Ar (FCC in 3D)

Physical example: Surface structures

- **Example**: Surface effects in some materials
- Need a description that includes the environment of an atom to model the bond strength between pairs of atoms



Pair potentials: All bonds are equal!



Reality: Have environment effects; it matter that there is a free surface!

MD updating scheme: Complete

(1) Updating method (integration scheme)

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

Positions at t_0-Δt | Positions at t_0 | Accelerations at t_0

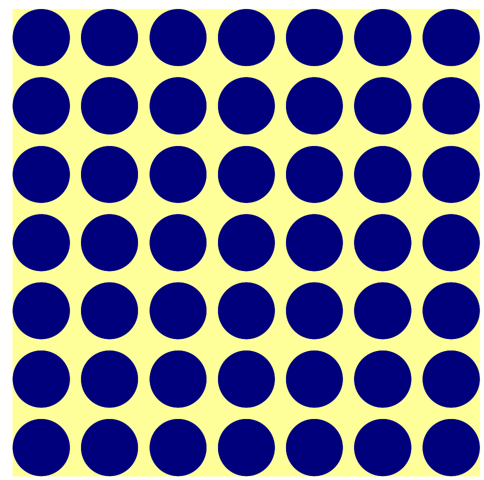
(2) Obtain accelerations from forces

"Verlet central difference method"

$$f_i = m a_i \qquad a_i = F_i / m$$

(5) Crystal (initial conditions)

Positions at t_0



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(3) Obtain forces from potential

$$F = -\frac{\mathrm{d}V(r)}{\mathrm{d}r} \qquad F_i = F\frac{x_i}{r}$$

(4) Potential

$$\phi_{weak}(r) = 4\varepsilon\left(\left[\frac{\sigma}{r}\right]^{12} - \left[\frac{\sigma}{r}\right]^{6}\right)$$

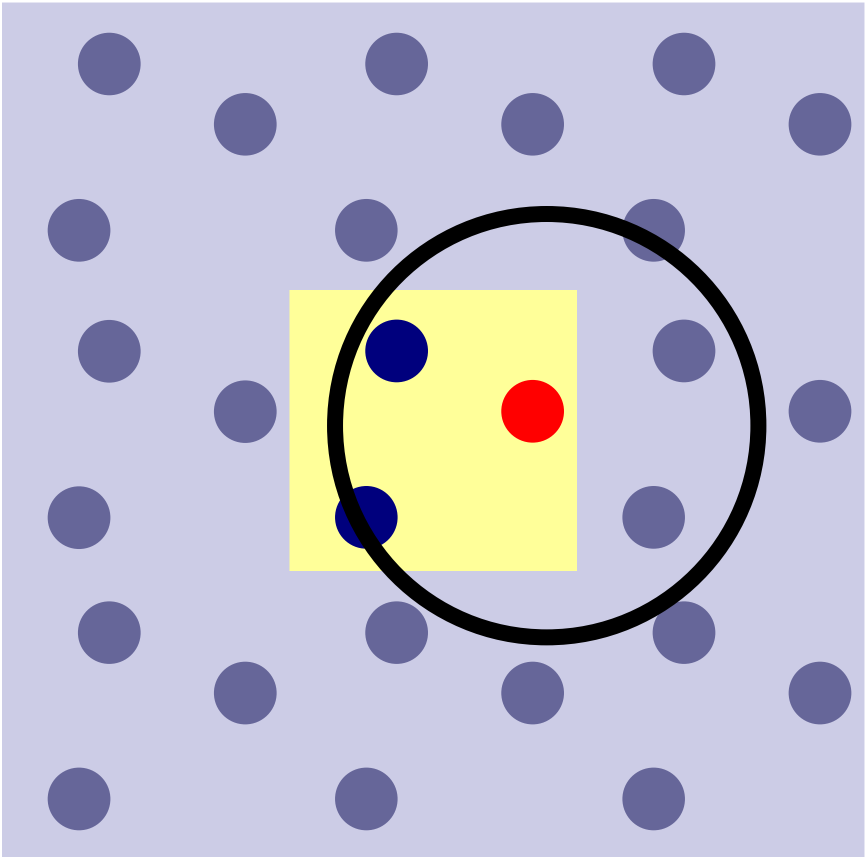
Neighbor lists

- Another bookkeeping device often used in MD simulation is a **Neighbor List** which keeps track of who are the nearest, second nearest, ... neighbors of each particle. This is to save time from checking every particle in the system every time a force calculation is made.
- The List can be used for several time steps before updating.

- Each update is expensive since it involves *N*x*N* operations for an *N*-particle system.

  In low-temperature solids where the particles do not move very much, it is possible to do an entire simulation without or with only a few updating, whereas in simulation of liquids, updating every 5 or 10 steps is quite common.

How are forces calculated?



Analysis methods

Last time, we discussed how to calculate:

- Temperature $T = \frac{2}{3}\frac{K}{N \cdot k_B}$ $K = \frac{1}{2} m \sum_{j=1}^{N} v_j^2$ Kinetic energy
- Potential energy $U = U(r_j)$
- Pressure $P = \underbrace{N/Vk_BT}_{\text{Kinetic contribution}} - \frac{1}{3V}\sum_i \sum_{j<i} \langle \underbrace{r_{ij}\frac{dV}{dr_{ij}}}\rangle$

Kinetic contribution

Volume

Force vector multiplied by distance vector

Time average

Need other measures for physical and thermodynamic properties

MD modeling of crystals: Challenges of data analysis

- 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.
- MD has become so well respected for what it can tell about the distribution of atoms and molecules in various states of matter, and the way they move about in response to thermal excitations or external stress such as pressure.

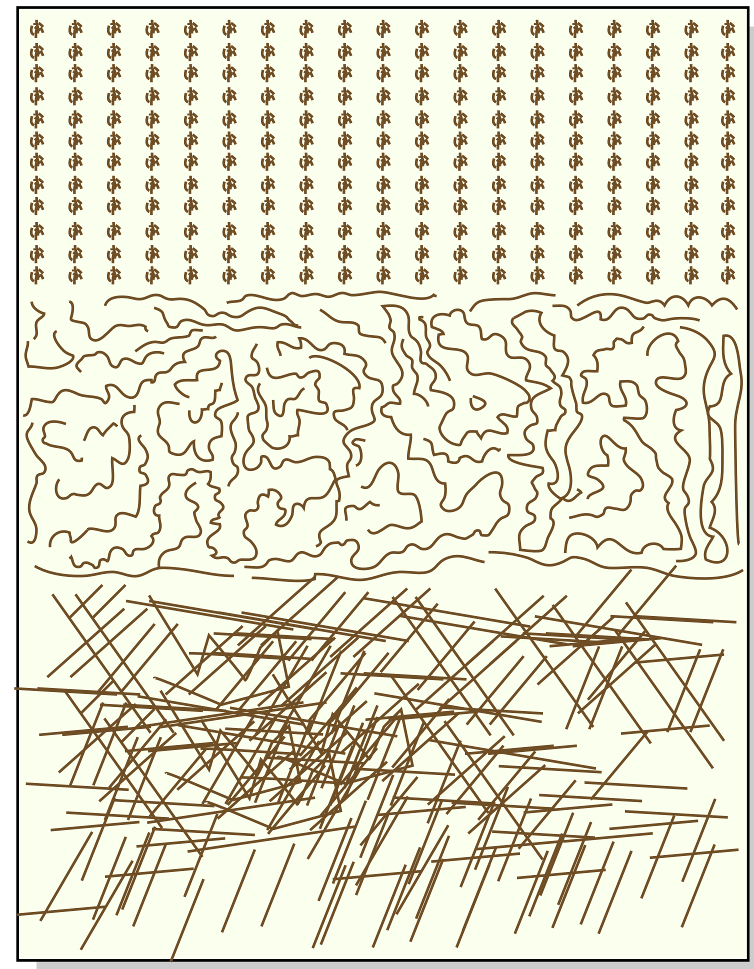


Figure by MIT OCW. After J. A. Barker and D. Henderson.

[J. A. Barker and D. Henderson, Scientific American, Nov. 1981].

Pressure, energy and temperature history

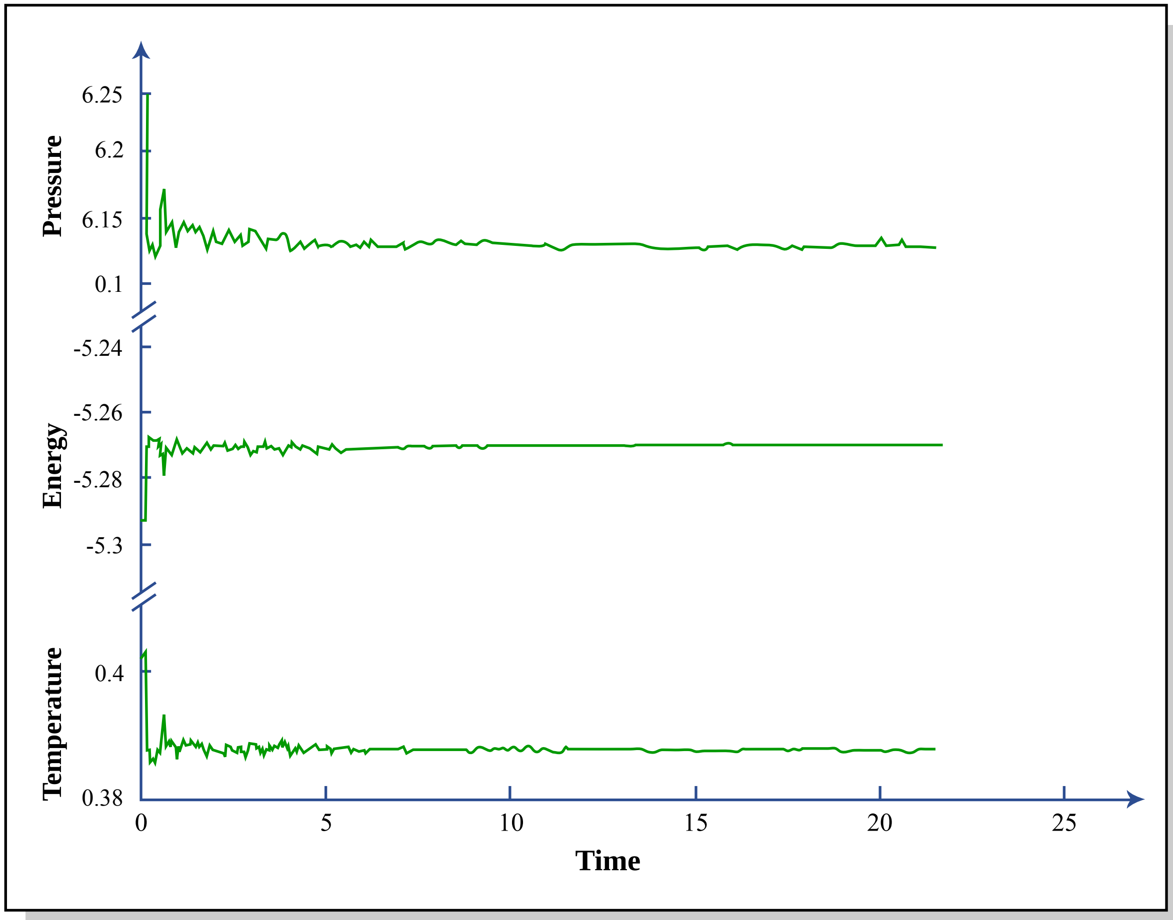


Figure by MIT OCW.

Time variation of system pressure, energy, and temperature in an MD simulation of a solid. The initial behavior are transients which decay in time as the system reaches equilibrium.

Pressure, energy and temperature history

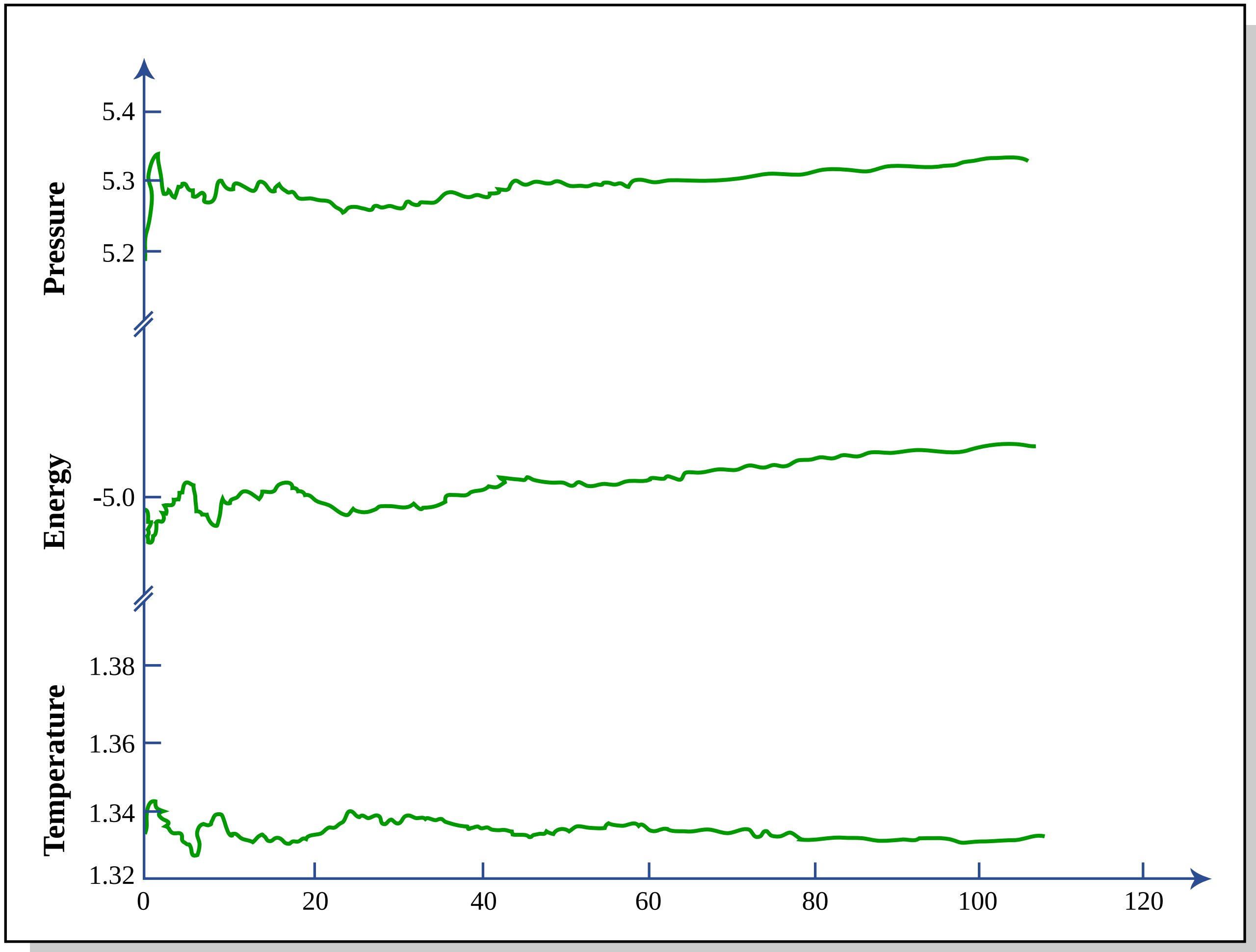


Figure by MIT OCW.

Time variation of system pressure, energy, and temperature in an MD simulation of a liquid: Longer transients

Analysis methods

Radial distribution function

The radial distribution function is defined as

Density of atoms (volume)

$$g(r) = \rho(r) / \rho$$

Local density

Provides information about the density of atoms at a given radius *r*; $\rho(r)$ is the local density of atoms

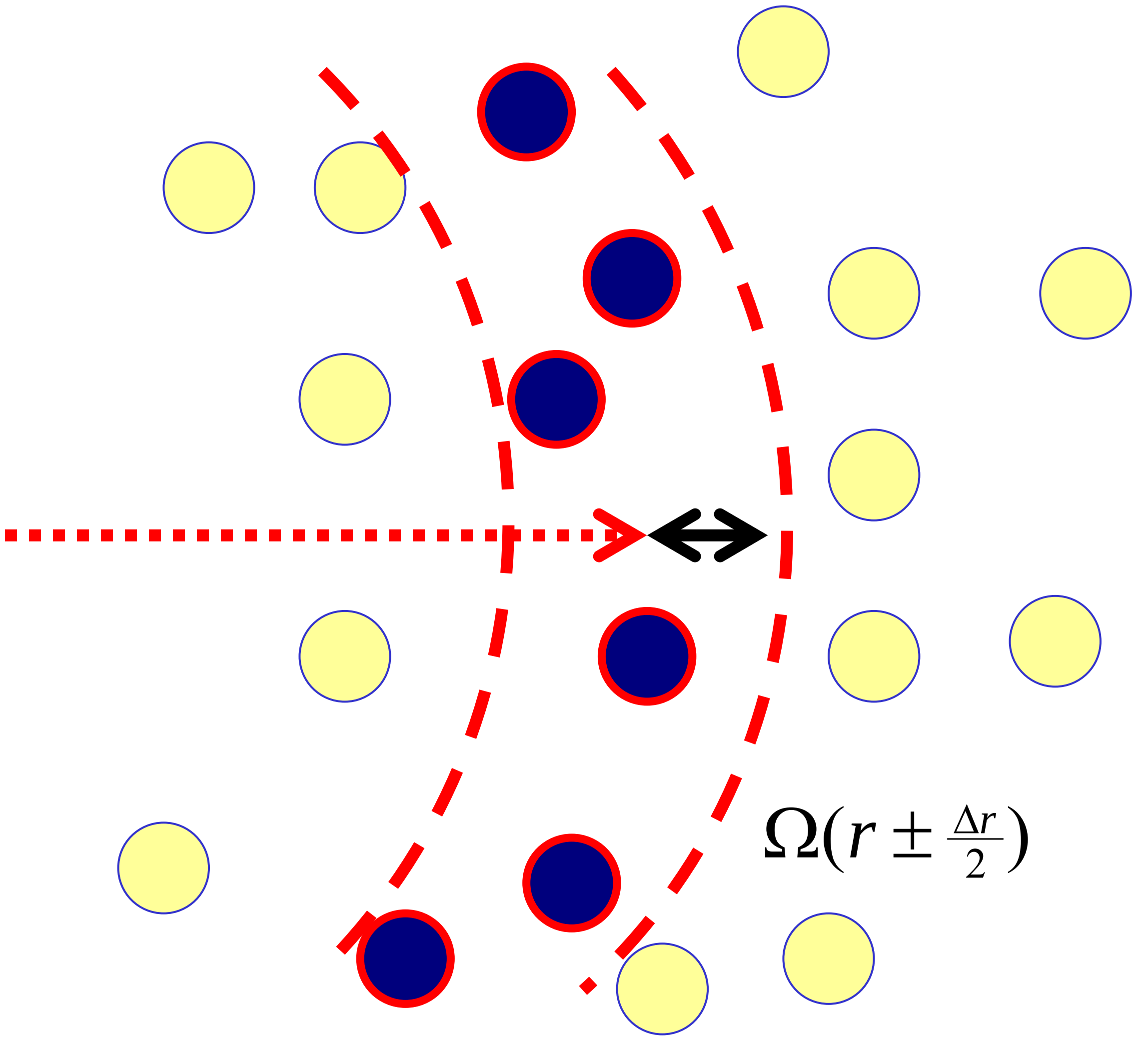
$$g(r) = \frac{< N(r \pm \frac{\Delta r}{2}) >}{\Omega(r \pm \frac{\Delta r}{2}) \rho}$$

→ Average over all atoms

Volume of this shell (dr)

$g(r) 2\pi r^2 dr =$ Number of particles lying in a spherical shell of radius *r* and thickness *dr*

Radial distribution function



considered volume

$$g(r) = \frac{N(r \pm \frac{\Delta r}{2})}{\Omega(r \pm \frac{\Delta r}{2})\rho}$$

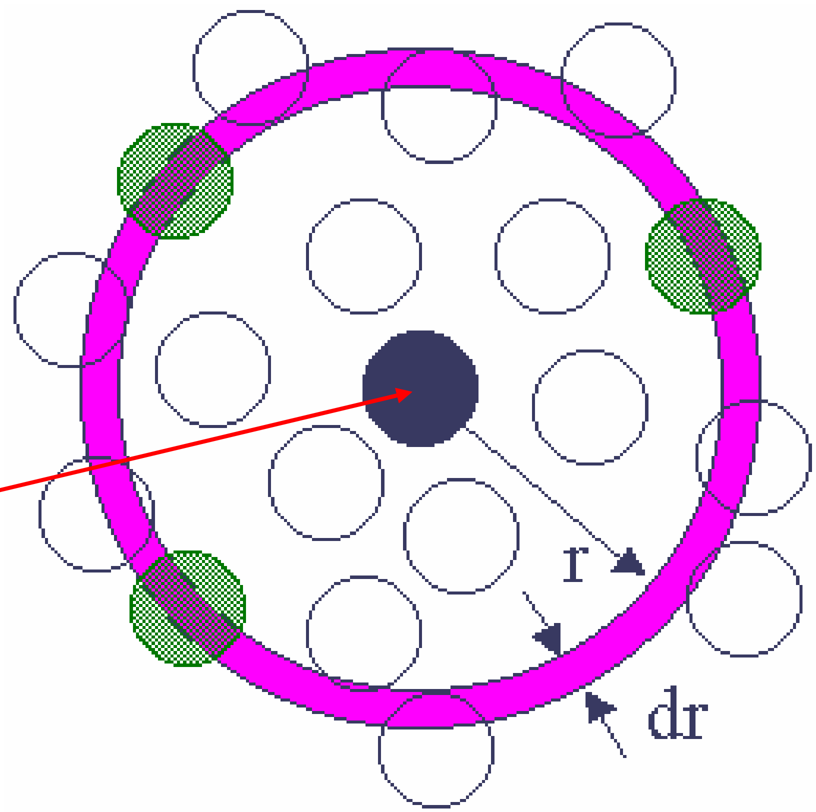
Particle density

$$\rho = N / V$$

Note: RDF can be measured experimentally using neutron-scattering techniques.

Radial distribution function

Reference atom



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http://www.ccr.buffalo.edu/etomica/app/modules/sites/Ljmd/Background1.html

Radial distribution function: Solid versus liquid

solid

liquid

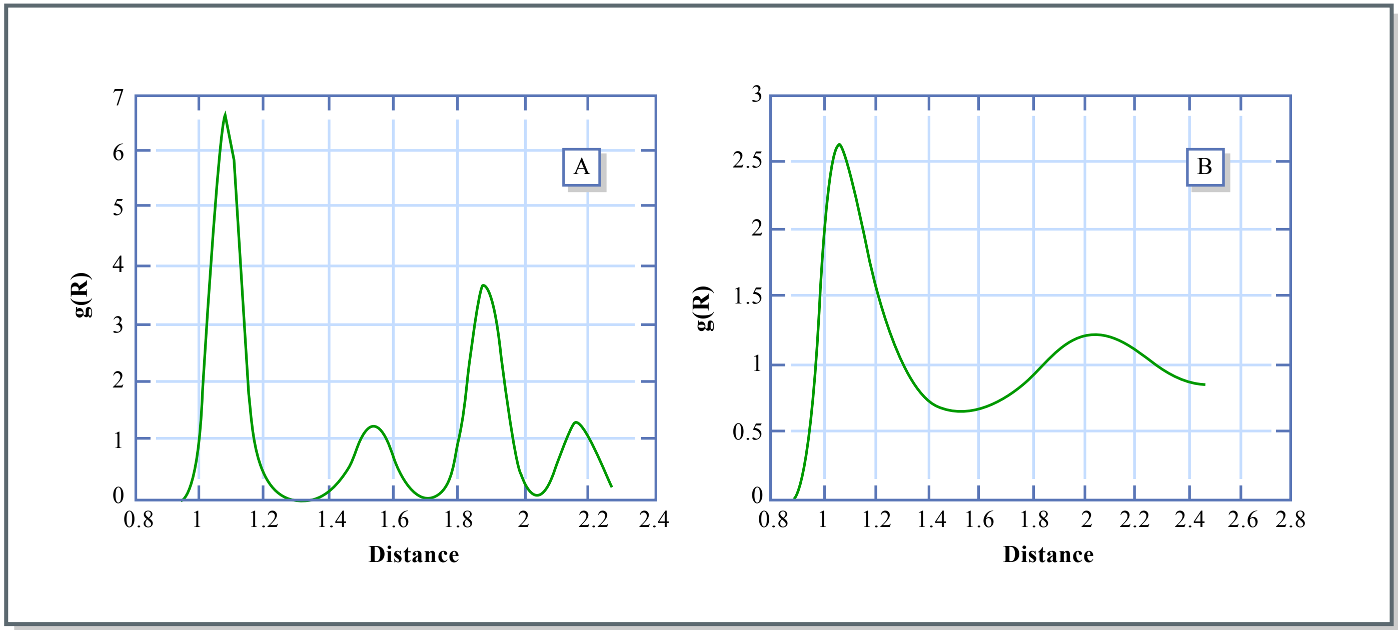


Figure by MIT OCW.

Interpretation: A peak indicates a particularly favored separation distance for the neighbors to a given particle

Thus: RDF reveals details about the atomic structure of the system being simulated

Java applet:
http://physchem.ox.ac.uk/~rkt/lectures/liqsolns/liquids.html

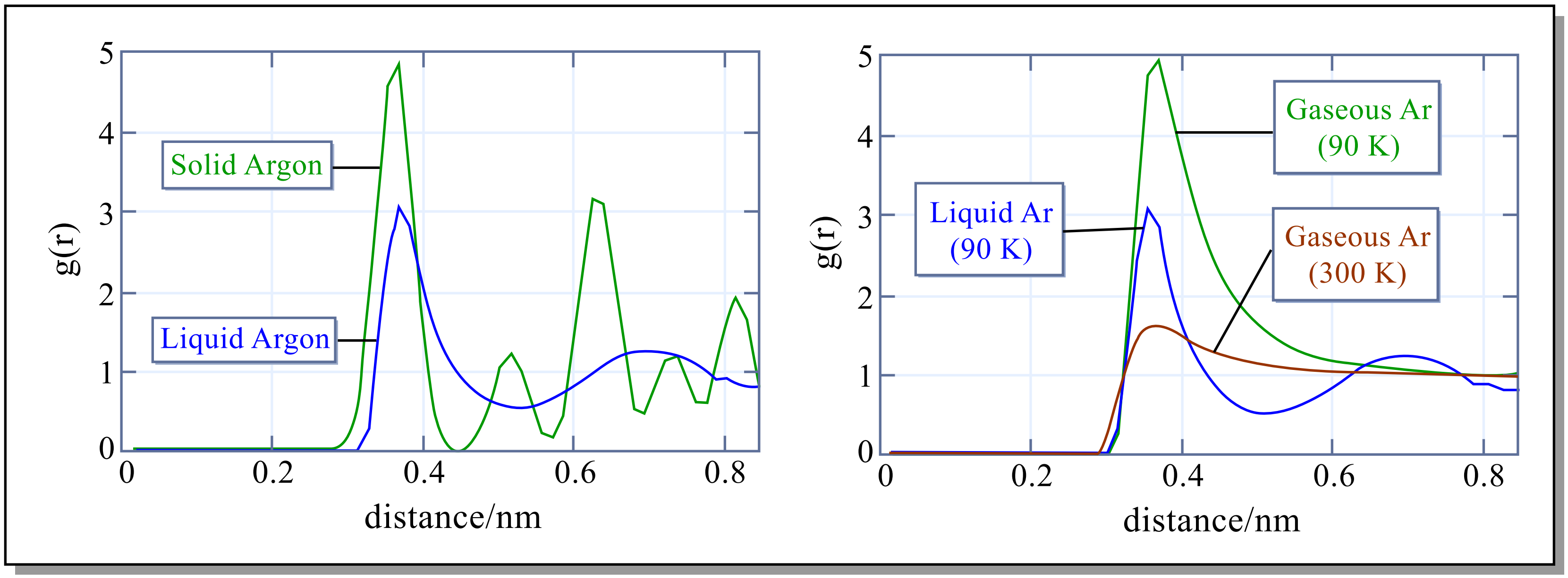
Radial distribution function: JAVA applet

Image removed for copyright reasons.
Screenshot of the radial distribution function Java applet.

Java applet:

http://physchem.ox.ac.uk/~rkt/lectures/liqsolns/liquids.html

Radial distribution function: Solid versus liquid versus gas



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Note: The first peak corresponds to the nearest neighbor shell, the second peak to the second nearest neighbor shell, etc.

In FCC: 12, 6, 24, and 12 in first four shells

Mean square displacement (MSD) function

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

If averaged over all particles: Mean square distance that particles have moved during time *t* *(measure of the average distance a molecule travels)*

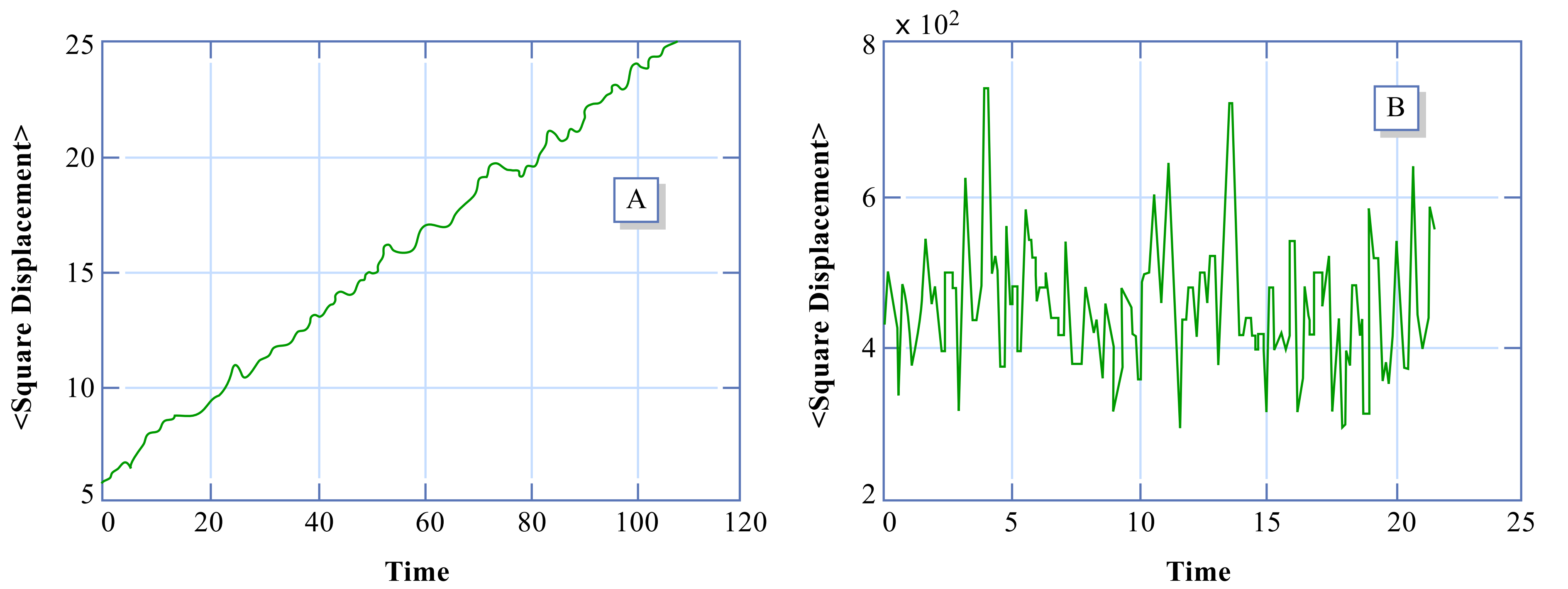
MSD is zero at t=0; grows like t^2 with a coefficient proportional to $k_B T/m$

Solid: Expect that MSD grows to a characteristic value (related to fluctuations around lattice site), then saturate

Liquid: All atoms diffuse continuously through the material, as in Brownian motion

Diffusion: Linear variation of MSD in time *t*

Mean square displacement (MSD) function



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Liquid

Crystal

Relation to diffusion constant:

$$\lim_{t\to\infty} \frac{d}{dt} < \Delta r^2 > = 2dD$$

d=2 2D

d=3 3D

Property calculation in MD

Time average of dynamical variable *A*(t)

$$< A >= \lim_{t\to\infty} \frac{1}{t} \int_{t'=0}^{t'=t} A(t')dt'$$

Time average of a dynamical variable *A*(*t*)

$$< A >= \frac{1}{N_t} \sum_{1}^{N_t} A(t)$$

Average over all time steps N_t in the trajectory (discrete)

Correlation function of two dynamical variables A(t) and B(t)

$$< A(0)B(t) >= \frac{1}{N} \sum_{i=1}^{N} \frac{1}{N_i} \sum_{k=1}^{N_i} A_i(t_k)B_i(t_k + t)$$

Overview: MD properties

$$U = < \sum_{i<j}^{N} V(r_{ij}) >$$ potential energy

$$T = \frac{1}{3Nk_B} < \sum_{i=1}^{N} m_i \underline{v}_i^2 >$$ temperature

$$P = \frac{1}{3V} < \sum_{i=1}^{N} (m_i \underline{v}_i^2 + \underline{r}_i \cdot \underline{f}_i) >$$ pressure

$$g(r) = \frac{1}{n 4\pi r^2 dr} < \sum_{i \neq j}^{N} \delta(r - |\underline{r}_i - \underline{r}_j|) >$$ radial distribution function

$$< \Delta r^2 > = \frac{1}{N} \sum_{i=1}^{N} [\underline{r}_i(t) - \underline{r}_i(0)]^2$$ mean squared displacement

Velocity autocorrelation function

$$< v(0)v(t) >= \frac{1}{N}\sum_{i=1}^{N}\frac{1}{N_i}\sum_{k=1}^{N_i} v_i(t_k)v_i(t_k+t)$$

•The velocity autocorrelation function gives information about the atomic motions of particles in the system

• Since it is a correlation of the particle velocity at one time with the velocity of the same particle at another time, the information refers to how a particle moves in the system, such as diffusion

Diffusion coeffecient (see e.g. Frenkel and Smit)**:**

$$D_0 = \frac{1}{3}\int_{t'=0}^{t'=\infty} < v(0)v(t) > dt'$$

Note: Belongs to the Green-Kubo relations can provide links between correlation functions and material transport coefficients, such as thermal conductivity, diffusivity etc.

Velocity autocorrelation function (VAF)

- **Liquid or gas (weak molecular interactions):**
  Magnitude reduces gradually under the influence of weak forces: Velocity decorrelates with time, which is the same as saying the atom 'forgets' what its initial velocity was.

  Then: VAF plot is a simple exponential decay, revealing the presence of weak forces slowly destroying the velocity correlation. Such a result is typical of the molecules in a gas.

- **Solid (strong molecular interactions):**
  Atomic motion is an oscillation, vibrating backwards and forwards, reversing their velocity at the end of each oscillation.
  Then: VAF corresponds to a function that oscillates strongly from positive to negative values and back again. The oscillations decay in time.

  This leads to a function resembling a damped harmonic motion.

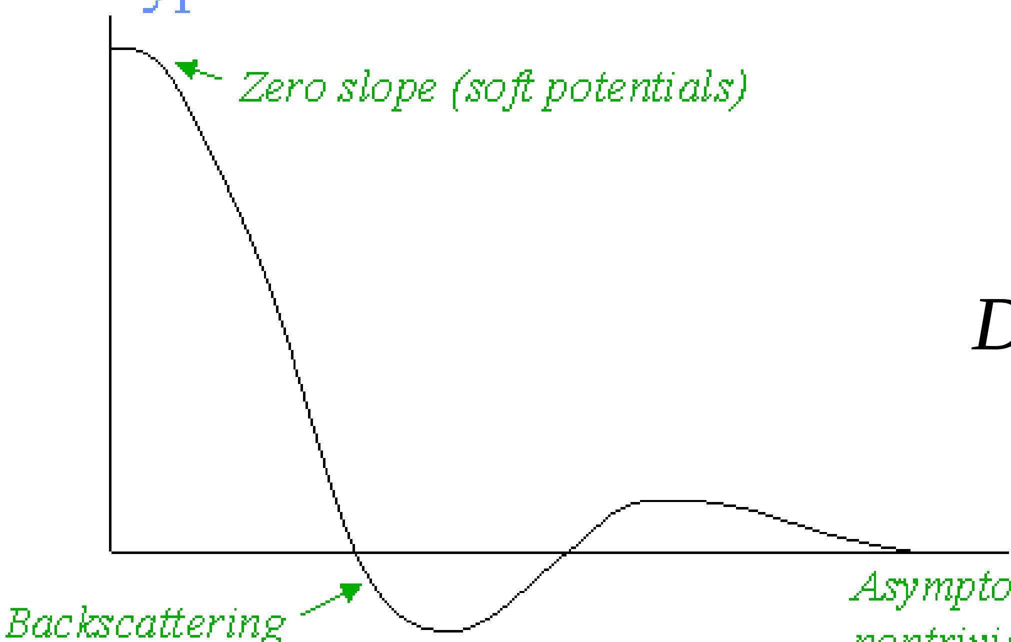
Velocity autocorrelation function

- Definition

$$C(t) \equiv \langle \mathbf{v}(0) \cdot \mathbf{v}(t) \rangle \qquad C(0) = \langle v^2 \rangle = dkT/m$$

solid

- Typical behavior



Diffusion constant is area under the curve

$$D_0 = \frac{1}{3} \int_{t'=0}^{t'=\infty} < v(0)v(t) > dt'$$

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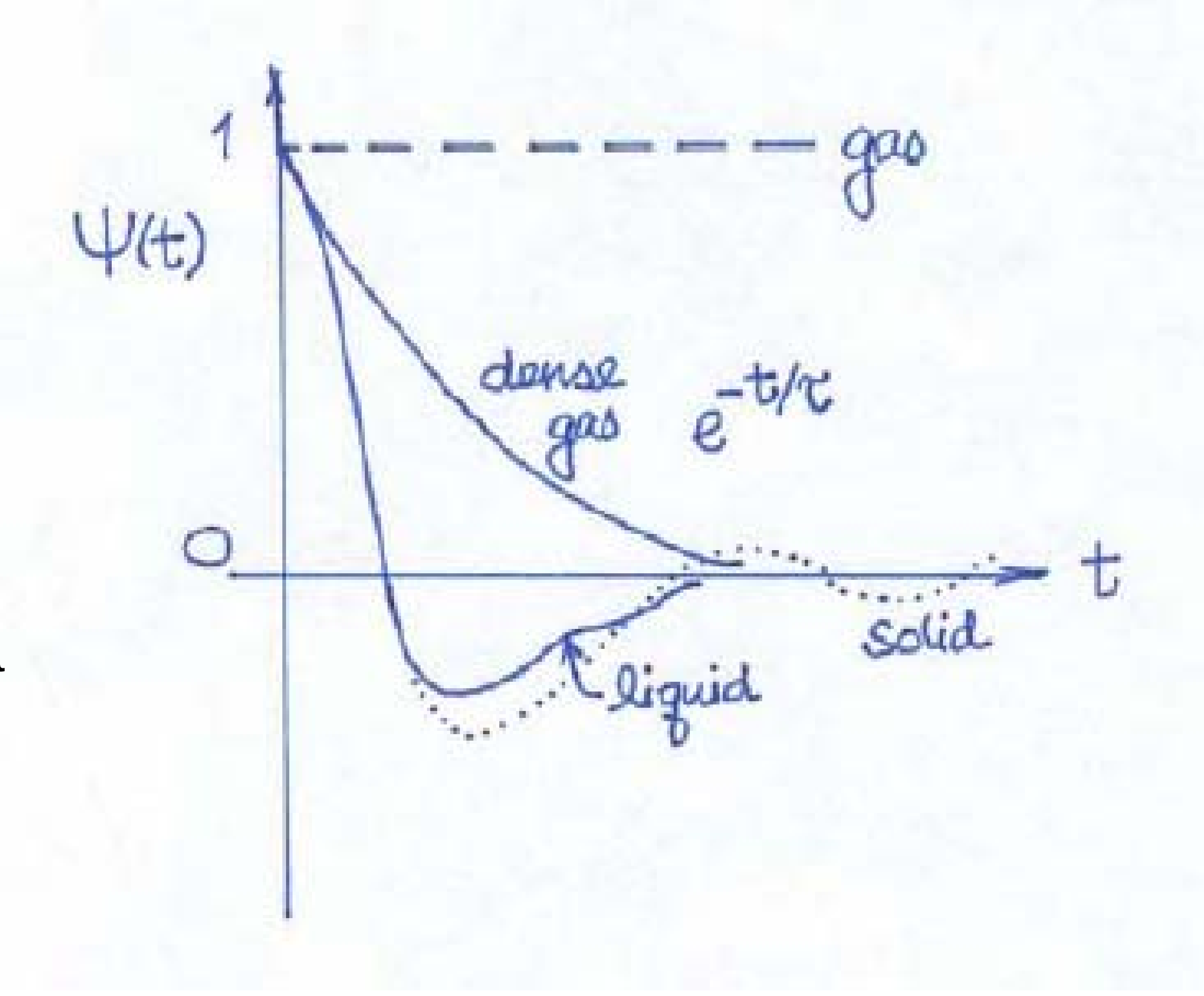
http://www.eng.buffalo.edu/~kofke/ce530/Lectures/Lecture12/sld010.htm

Velocity autocorrelation function

The velocity autoccorelation function for an ideal gas, a dense gas, a liquid, and a solid



The concept of stress

Undeformed
vs. deformed
(due to force)

$$\sigma = \frac{F}{A}$$

A = cross-sectional area

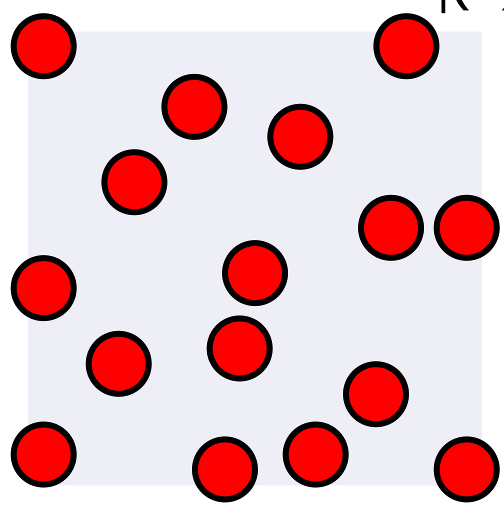
Atomic stress tensor: Cauchy stress

- How to relate the continuum stress with atomistic stress

- Typically continuum variables represent time-/space averaged microscopic quantities at equilibrium
- Difference: Continuum properties are valid at a specific material point; this is not true for atomistic quantities (discrete nature of atomic microstructure)

Continuous fields $u_i(x)$

Discrete fields $u_i(x)$



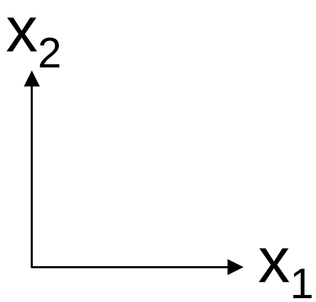
Displacement only defined at atomic site

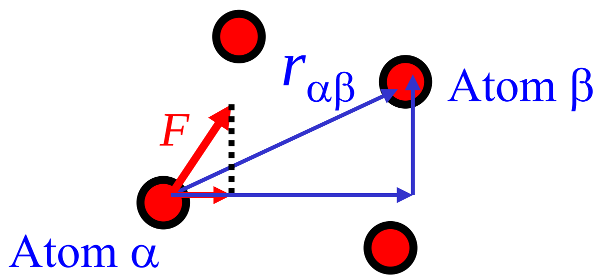
Atomic stress tensor: Virial stress

Virial stress:

Contribution by atoms moving through control volume

$$\sigma_{ij} = \frac{1}{\Omega}\left(-\sum_{\alpha} m_{\alpha} u_{\alpha,i} u_{\alpha,j} + \frac{1}{2}\sum_{\alpha,\beta,a\neq\beta} \underbrace{\frac{\partial \phi(r)}{\partial r}\frac{r_i}{r}}_{\text{Force } F_i} \cdot r_j \,\Big|_{r=r_{\alpha\beta}}\right)$$





http://ej.iop.org/links/q12/tWFV6mZig3VMoH,nK2DO8w/nano3_11_009.pdf
http://ej.iop.org/links/q67/dpRsM7WvMemOvng7LbbU7A/msmse4_4_S03.pdf

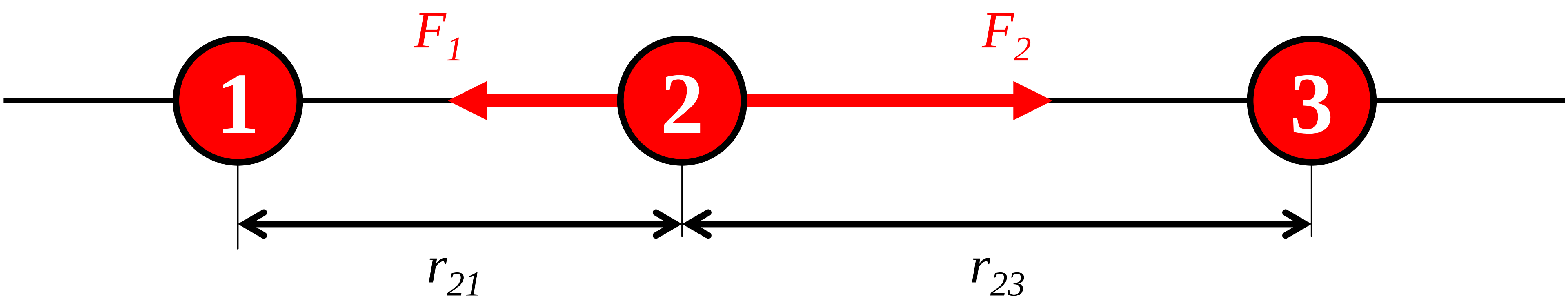
D.H. Tsai. Virial theorem and stress calculation in molecular-dynamics. *J. of Chemical Physics*, 70(3):1375–1382, 1979.

Min Zhou, A new look at the atomic level virial stress: on continuum-molecular system equivalence, Royal Society of London Proceedings Series A, vol. 459, Issue 2037, pp.2347-2392 (2003)

Jonathan Zimmerman *et al*., Calculation of stress in atomistic simulation, MSMSE, Vol. 12, pp. S319-S332 (2004) and references in those articles by Yip, Cheung *et al.*

Virial stress in 1D

$$\sigma_{ij} = \frac{1}{\Omega}\left(-\sum_{\alpha} m_\alpha u_{\alpha,i} u_{\alpha,j} + \frac{1}{2}\sum_{\alpha,\beta,a\neq\beta} \frac{\partial\phi(r)}{\partial r}\frac{r_i}{r}\cdot r_j \Big|_{r=r_{\alpha\beta}} \right)$$



$$\sigma_{ij} = \frac{1}{\Omega}\frac{1}{2}\sum_{\alpha,\beta,a\neq\beta} \frac{\partial\phi(r)}{\partial r}\frac{r_i}{r}\cdot r_j \Big|_{r=r_{\alpha\beta}}$$

Force between 2 particles:

$$F = -\frac{\partial\phi(r)}{\partial r}\frac{r_i}{r}$$

$$\sigma_{11} = \frac{1}{\Omega}\frac{1}{2}\left(F_1 r_{21} + F_2 r_{23}\right)$$

Other transport properties

Diffusivity

$$D = \frac{1}{Vd\rho}\int_0^\infty dt \left\langle \mathbf{v}(0)\cdot\mathbf{v}(t)\right\rangle \qquad \mathbf{v} = \sum_{i=1}^{N}[\mathbf{v}_i]$$

Shear viscosity

$$\eta = \frac{1}{VkT}\int_0^\infty dt \left\langle \sigma^{xy}(t)\sigma^{xy}(0)\right\rangle \qquad \sigma^{xy} = \sum_{i=1}^{N}\left[m_i v_i^x v_i^y + \frac{1}{2}\sum_{i\neq j} x_{ij} f_y(r_{ij})\right]$$

Thermal conductivity

$$\lambda_T = \frac{1}{VkT^2}\int_0^\infty dt \left\langle q(t)q(0)\right\rangle \qquad q = \frac{d}{dt}\sum_{i=1}^{N}\left[\frac{1}{2}m_i v_i^2 + \frac{1}{2}\sum_{i\neq j} u(r_{ij})\right]$$

http://www.cbe.buffalo.edu/courses/ce530/Lectures/Lecture12/sld011.htm

MD properties: Classification

- Structural – crystal structure, *g*(r), defects such as vacancies and interstitials, dislocations, grain boundaries, precipitates
- Thermodynamic -- equation of state, heat capacities, thermal expansion, free energies
- Mechanical -- elastic constants, cohesive and shear strength, elastic and plastic deformation, fracture toughness
- Vibrational -- phonon dispersion curves, vibrational frequency spectrum, molecular spectroscopy
- Transport -- diffusion, viscous flow, thermal conduction

Modeling vs. simulation

- **Modeling**: Building a mathematical or theoretical description of a physical situation; maybe result in a set of partial differential equations

  For MD: Choice of potential, choice of crystal structure,…

- **Simulation**: Numerical solution of the problem at hand (code, infrastructure..)

  Solve the equations – e.g. Verlet method, parallelization (later)

- Simulation usually requires analysis methods – postprocessing (RDF, temperature…)

Limitations of MD: Electronic properties

- There are properties which classical MD cannot calculate because electrons are involved.

- To treat electrons properly one needs quantum mechanics. In addition to electronic properties, optical and magnetic properties also require quantum mechanical (first principles or *ab initio*) treatments.

What makes MD unique…

- Unified study of all physical properties.

  Using MD one can obtain thermodynamic, structural, mechanical, dynamic and transport properties of a system of particles which can be a solid, liquid, or gas.

  One can even study chemical properties and reactions which are more difficult and will require using quantum MD.

(adapted from Sid. Yip, Nuclear Engrg./MIT)

What makes MD unique…

- Several hundred particles are sufficient to simulate bulk matter.

  While this is not always true, it is rather surprising that one can get quite accurate thermodynamic properties such as equation of state in this way.

  This is an example that the law of large numbers takes over quickly when one can average over several hundred degrees of freedom.

(adapted from Sid. Yip, Nuclear Engrg./MIT)

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- Direct link between potential model and physical properties.

  This is really useful from the standpoint of fundamental understanding of physical matter.

  It is also very relevant to the structure-property correlation paradigm in materials science.

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What makes MD unique…

- Detailed atomic trajectories.

  This is what one can get from MD, or other atomistic simulation techniques, that experiment often cannot provide.

  This point alone makes it compelling for the experimentalist to have access to simulation.

(adapted from Sid. Yip, Nuclear Engrg./MIT)

Summary

- Discussed additional analysis techniques: “How to extract useful information from MD results”
  - Velocity autocorrelation function
  - Atomic stress
  - Radial distribution function …

- These are useful since they provide quantitative information about molecular structure in the simulation; e.g. during phase transformations, how atoms diffuse, elastic (mechanical) properties …

- Discussed some “simple” interatomic potentials that describe the atomic interactions; “condensing out” electronic degrees of freedom

- Elastic properties: Calculate response to mechanical load based on “virial stress”

- Briefly introduced the “training” of potentials – *homework assignment*

Ductile versus brittle materials

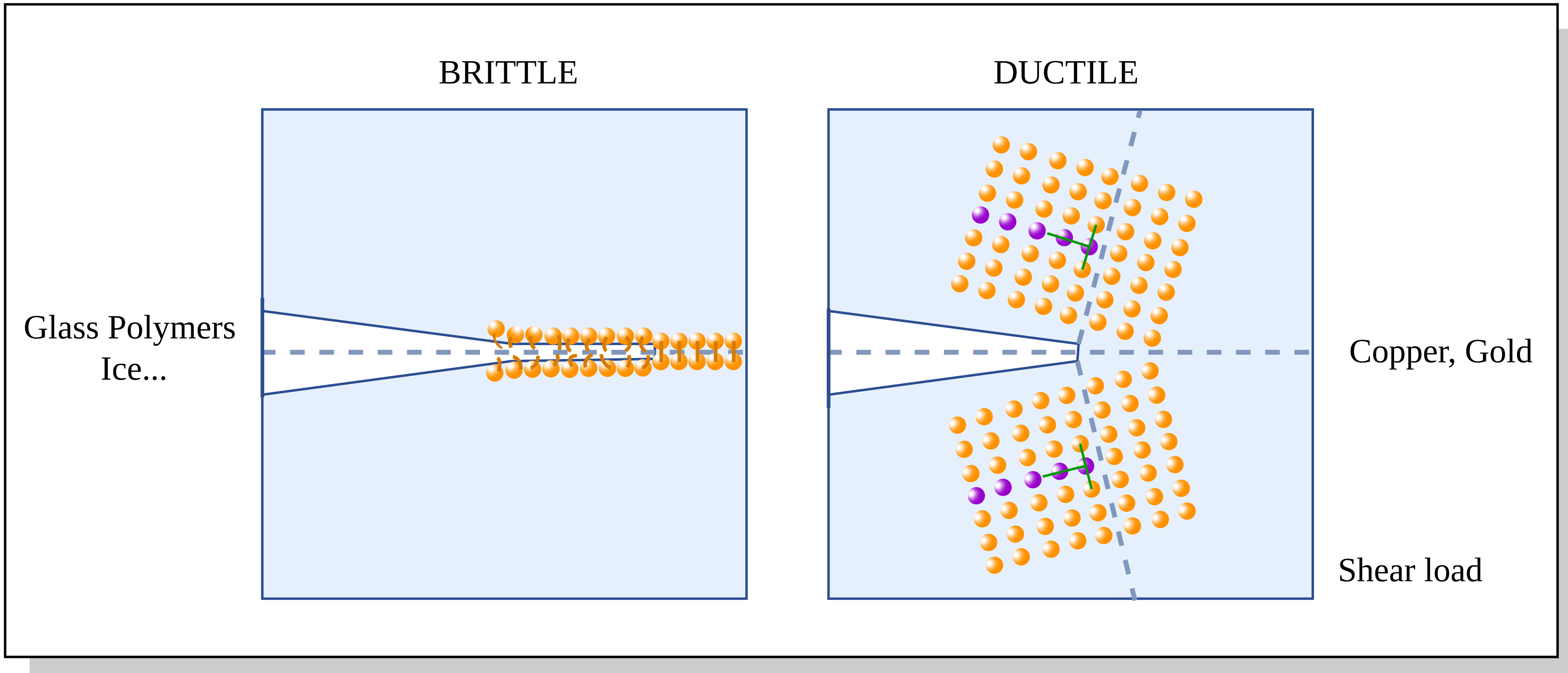
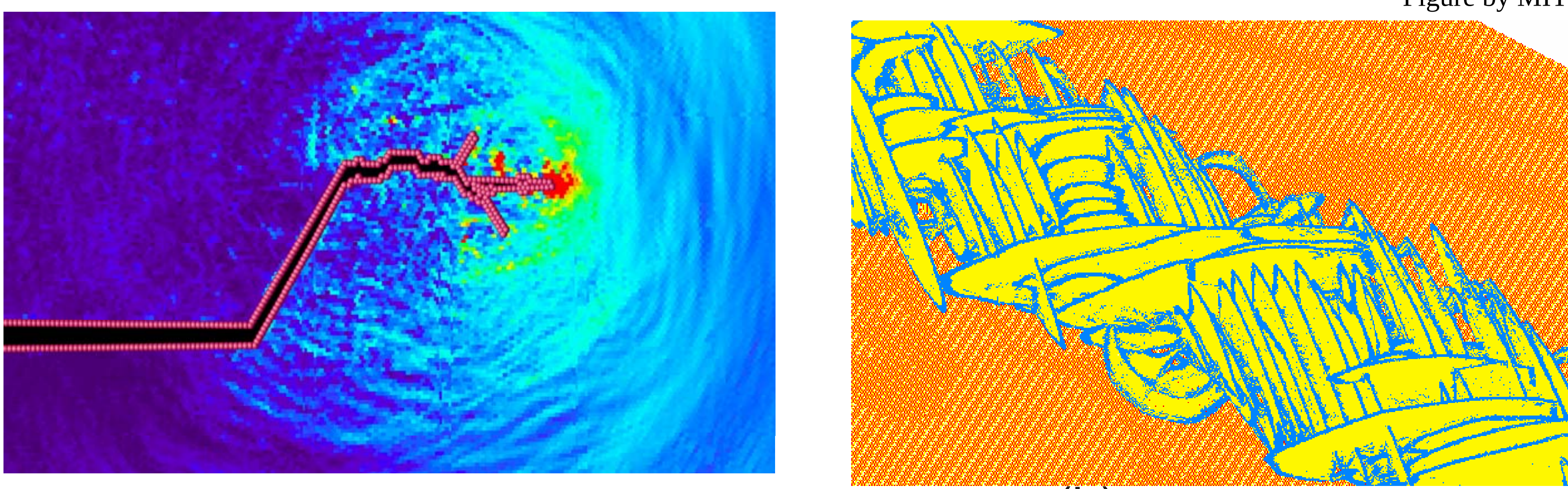


Figure by MIT OCW.



(a) (b)

Deformation of metals: Example

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See: Fig. 4 at http://www.kuleuven.ac.be/bwk/materials/Teaching/master/wg02/l0310.htm.

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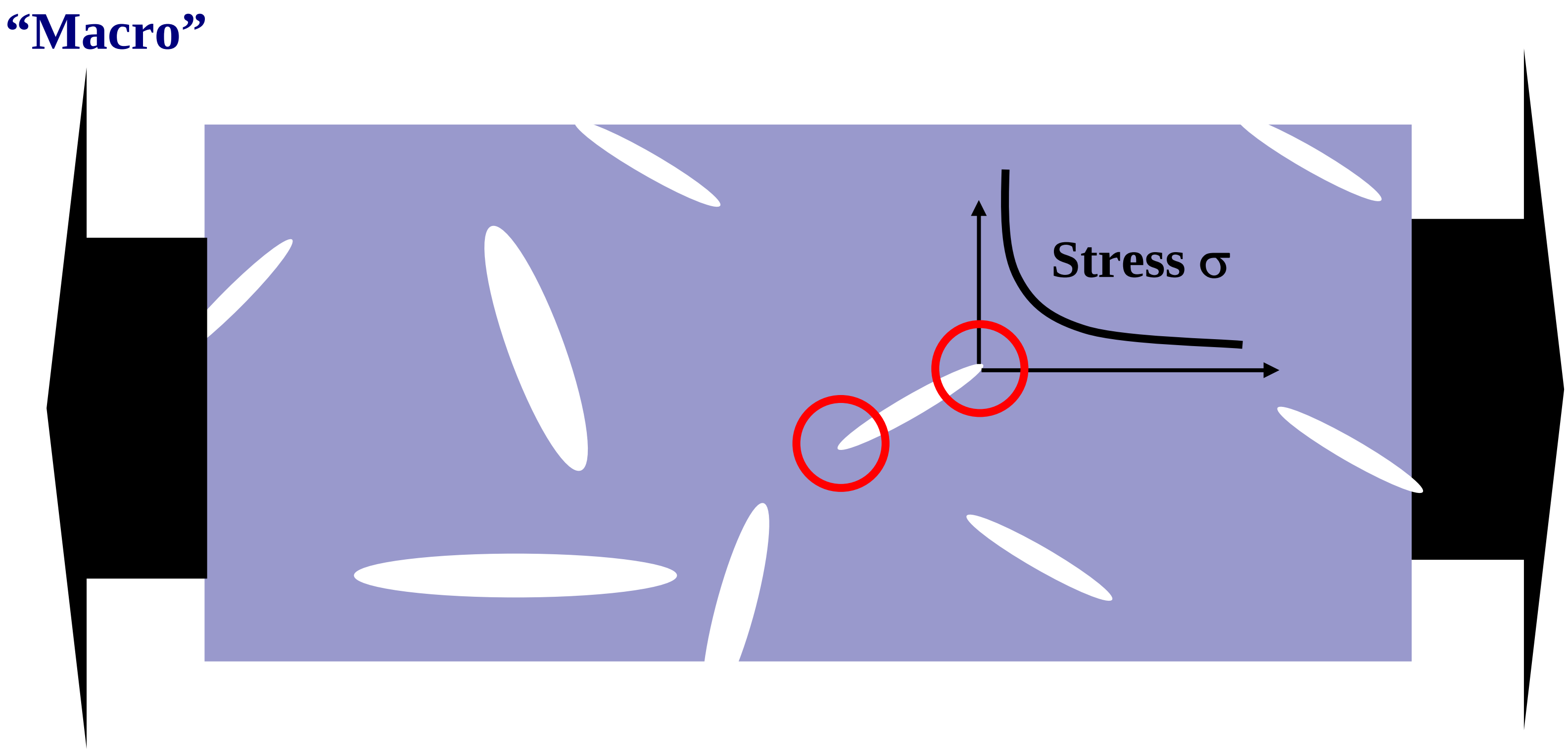
See: Fig. 6 at http://www.kuleuven.ac.be/bwk/materials/Teaching/master/wg02/l0310.htm.

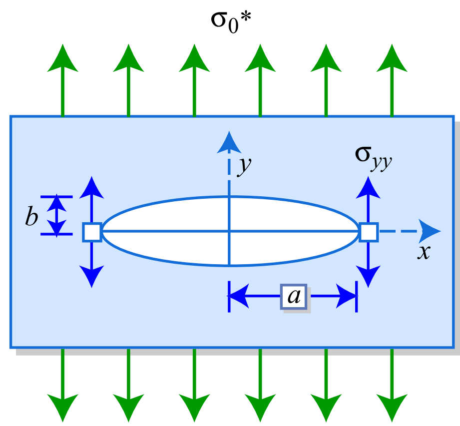
Deformation of materials: Flaws or cracks matter



Failure of materials initiates at cracks

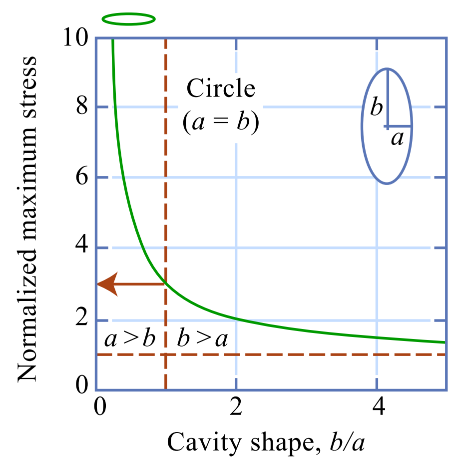
Griffith, Irwine and others: Failure initiates at defects, such as cracks, or grain boundaries with reduced traction, nano-voids

Inglis' solution: Elliptical hole and hole



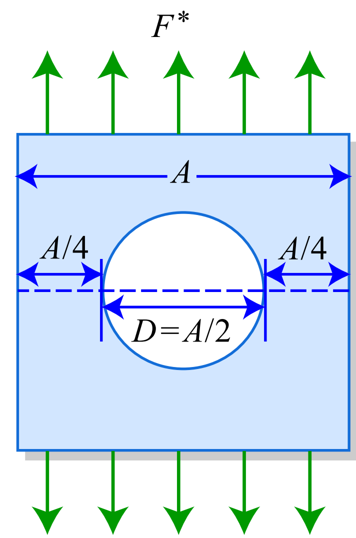
Model setup for the Inglis/Kolosov problem.

Figure by MIT OCW.



Plot of stress changes at the edge of elliptical cavities. Normalized maximum stress is σ_{yy}/σ_0^*; insets at top show ellipse orientations. The dashed horizontal line shows the level of stress change in the plate without a cavity present. Arrow shows stress concentration (3.0) for the circular hole ($a = b$).

Figure by MIT OCW.



Geometry for calculating stress in a plate with a circular hole.

Figure by MIT OCW.

$$\sigma_{yy} = \sigma_0^* \left(1 + 2\frac{a}{b} \right)$$

$$\sigma_{yy} = \sigma_0^* \left(1 + 2\sqrt{\frac{a}{\rho}} \right)$$

Stress magnification