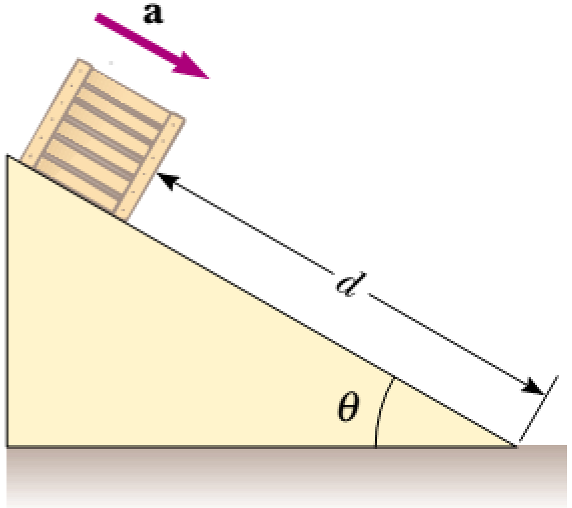
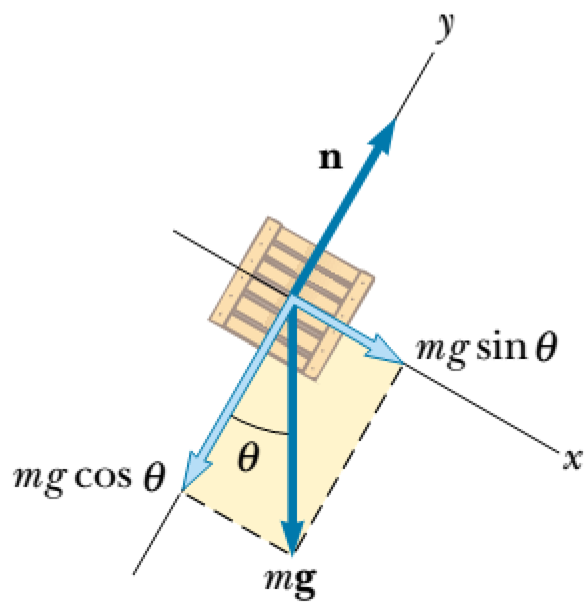
Overview of Thermodynamics

Newton's Second Law

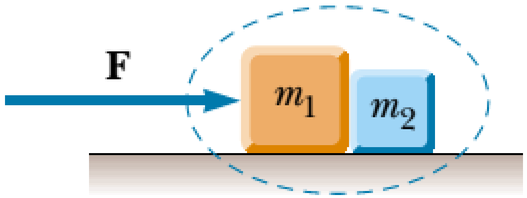




$$\sum \mathbf{F} = m\mathbf{a}$$

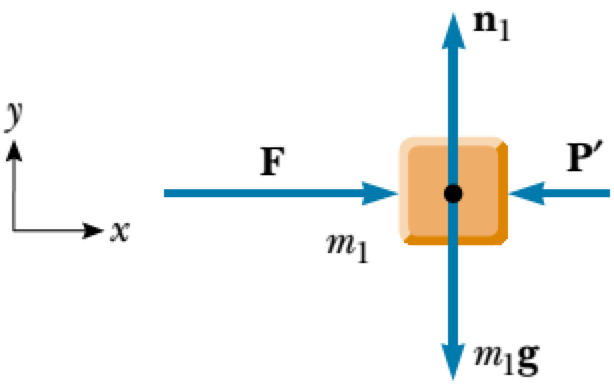
The acceleration of an object is directly proportional to the net force acting on it and inversely proportional to its mass.

Two-Block Problem

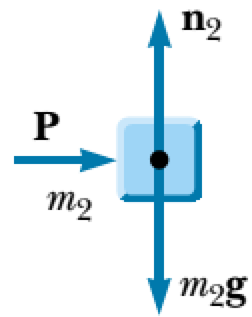


(a)

$$\sum F_x(\text{system}) = F = (m_1 + m_2)\,a_x$$



(b)



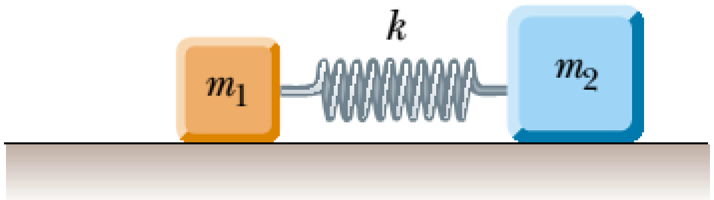
(c)

$$\sum F_x = P = m_2 a_x$$

$$P = m_2 a_x = \left(\frac{m_2}{m_1 + m_2}\right)F$$

Common sense tells us that both blocks must experience the same acceleration because they remain in contact with each other.

One, Two, Many



$$x_{\mathrm{CM}} \equiv \frac{m_1 x_1 + m_2 x_2}{m_1 + m_2}$$

$$x_{\mathrm{CM}} \equiv \frac{m_1 x_1 + m_2 x_2 + m_3 x_3 + \cdots + m_n x_n}{m_1 + m_2 + m_3 + \cdots + m_n} = \frac{\sum_i m_i x_i}{\sum_i m_i}$$

$$\mathbf{r}_{\mathrm{CM}} \equiv \frac{\sum_i m_i \mathbf{r}_i}{M} \longrightarrow \boxed{\mathbf{r}_{\mathrm{CM}} = \frac{1}{M}\int \mathbf{r}\, dm}$$

One, Two, Many

$$\mathbf{r}_{\mathrm{CM}} \equiv \frac{\sum_i m_i \mathbf{r}_i}{M}$$

$$\mathbf{v}_{\mathrm{CM}} = \frac{d\mathbf{r}_{\mathrm{CM}}}{dt} = \frac{1}{M}\sum_i m_i \frac{d\mathbf{r}_i}{dt} = \frac{\sum_i m_i \mathbf{v}_i}{M} \qquad M\mathbf{v}_{\mathrm{CM}} = \sum_i m_i \mathbf{v}_i = \sum_i \mathbf{p}_i = \mathbf{p}_{\mathrm{tot}}$$

$$\mathbf{a}_{\mathrm{CM}} = \frac{d\mathbf{v}_{\mathrm{CM}}}{dt} = \frac{1}{M}\sum_i m_i \frac{d\mathbf{v}_i}{dt} = \frac{1}{M}\sum_i m_i \mathbf{a}_i$$

$$M\mathbf{a}_{\mathrm{CM}} = \sum_i m_i \mathbf{a}_i = \sum_i \mathbf{F}_i \longrightarrow \boxed{\sum \mathbf{F}_{\mathrm{ext}} = M\mathbf{a}_{\mathrm{CM}} = \frac{d\mathbf{p}_{\mathrm{tot}}}{dt}}$$

The center of mass of a system of particles of combined mass M moves like an equivalent particle of mass M would move under the influence of the resultant external force on the system.

The Road Behind

Already learned:

- **Single-particle mechanics:**

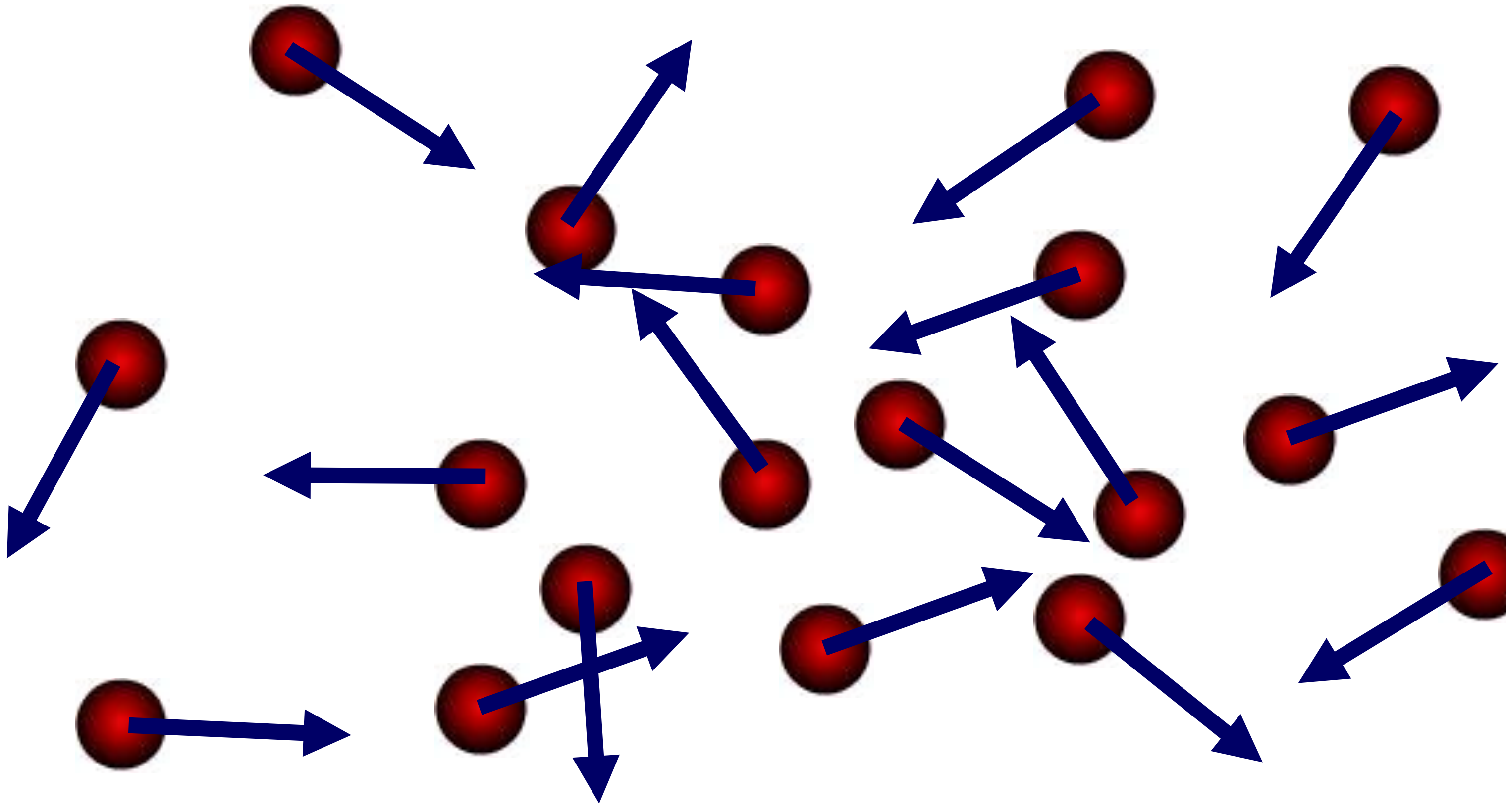
  translational and rotational variables
- **Two particles:**

  center of mass + relative motion
- **Many particles: center-of-mass translation**
  - **Rigid bodies: also rotation about a fixed axis**
  - **Realistic solids: vibrations**

Fluids: gases, liquids

The Naïve Approach

N particles $r_i(t)$, $v_i(t)$; interaction $V(r_i - r_j)$



A Simple Algorithm

Time-step propagator

$$U_F(\Delta t)\begin{pmatrix} x \\ v \end{pmatrix} = \begin{pmatrix} x \\ v + (F(x)/m)\Delta t \end{pmatrix}$$

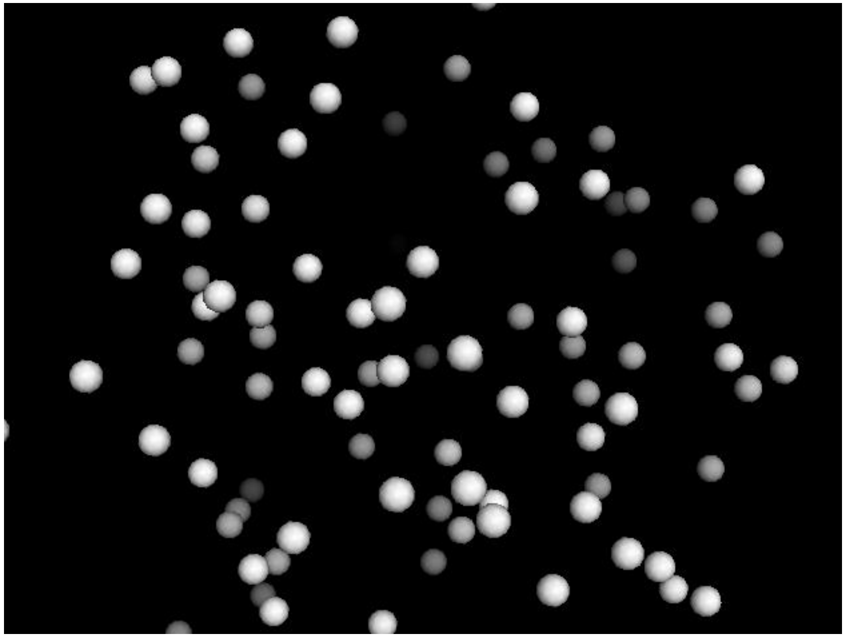
$$U_v(\Delta t)\begin{pmatrix} x \\ v \end{pmatrix} = \begin{pmatrix} x + v\Delta t \\ v \end{pmatrix}$$

Apply $U_F(\frac{1}{2}\Delta t)\,U_v(\Delta t)\,U_F(\frac{1}{2}\Delta t)$ to $x(t_n), v(t_n)$. This yields

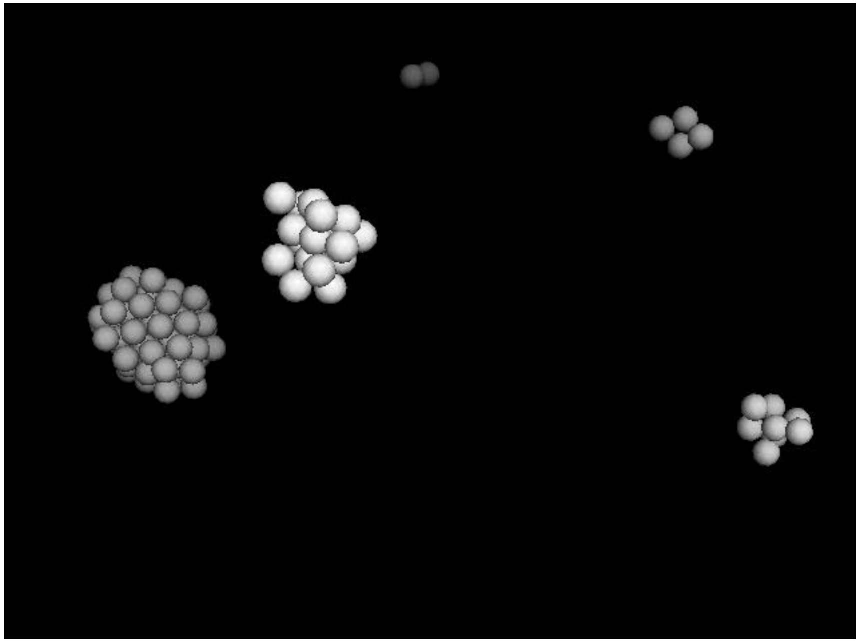
$$v_{n+1} = v_n + \frac{1}{2m}F_n\Delta t + \frac{1}{2m}F_{n+1}\Delta t$$

$$x_{n+1} = x_n + (v_n + \frac{1}{2m}F_n\Delta t)\Delta t$$

MD Simulation (Argon)

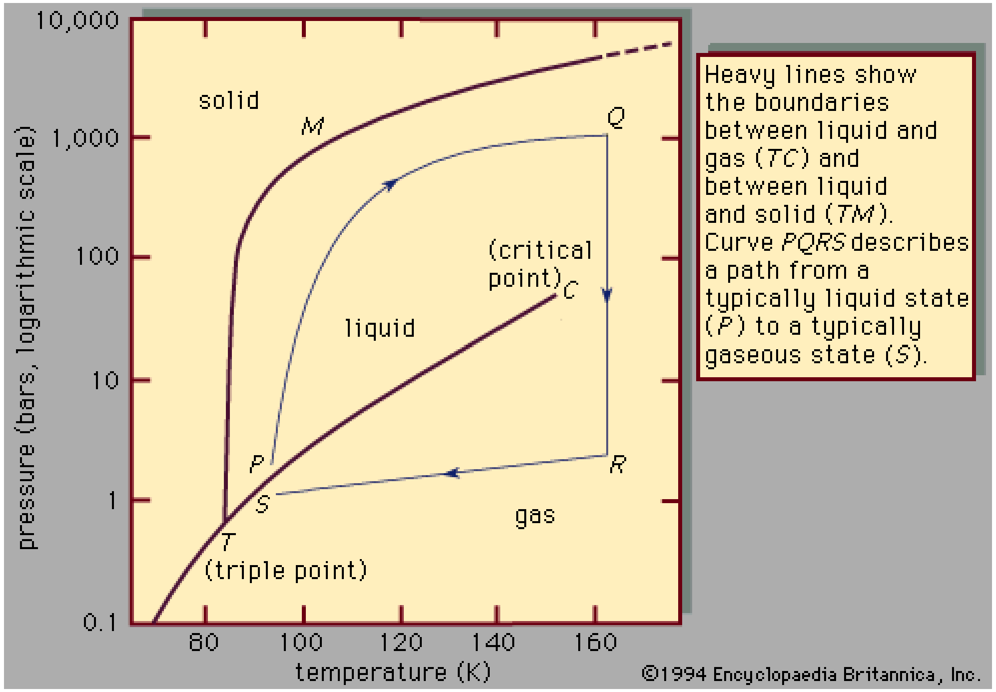


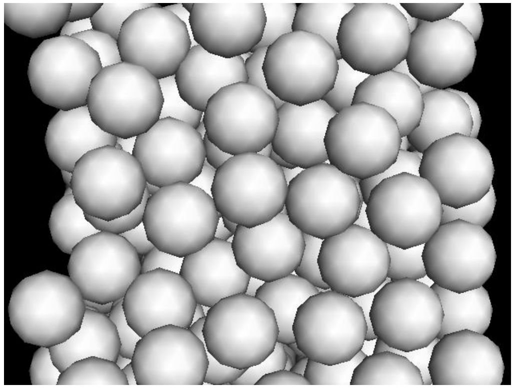
100 K (above the boiling point)

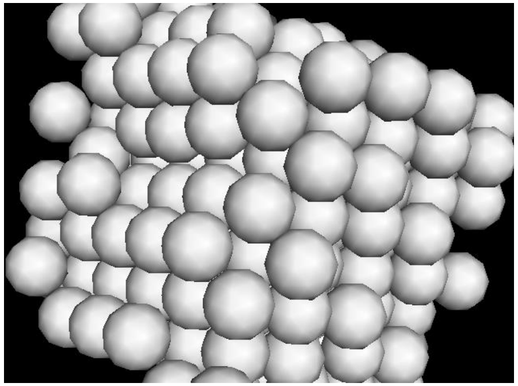


25 K (below the melting point)

Liquid Argon Freezing







Definitions

States of matter: phases

- **Gases: e.g., water vapor, oxygen**
- **Liquids: e.g., water, blood, mercury**
- **Solids: e.g., ice, glacier, rock, rubber**

"… physicist rejects the definition of a solid as (roughly) what hurts your toe when you kick it …"

-- *Concepts in Solids*, by P.W. Anderson

Comparison of Phases

	Solid	Liquid	Gas
Compression	Difficult	Difficult	Easy
Tension	Strong	Limited	No
Shear force	Normally, sustainable	Not sustainable	Not sustainable
Change shape?	Normally, no	Easily	Easily
Intermolecular forces	Strong	Relatively weak	Very weak

By Rigidity

- **Fluids [*Latin*, to flow]: liquids & gases**
  - **Flow to take the shape of container**
- **Normally, solids do not flow**

Statics: fluids at rest

Dynamics: fluids in motion

By Interaction

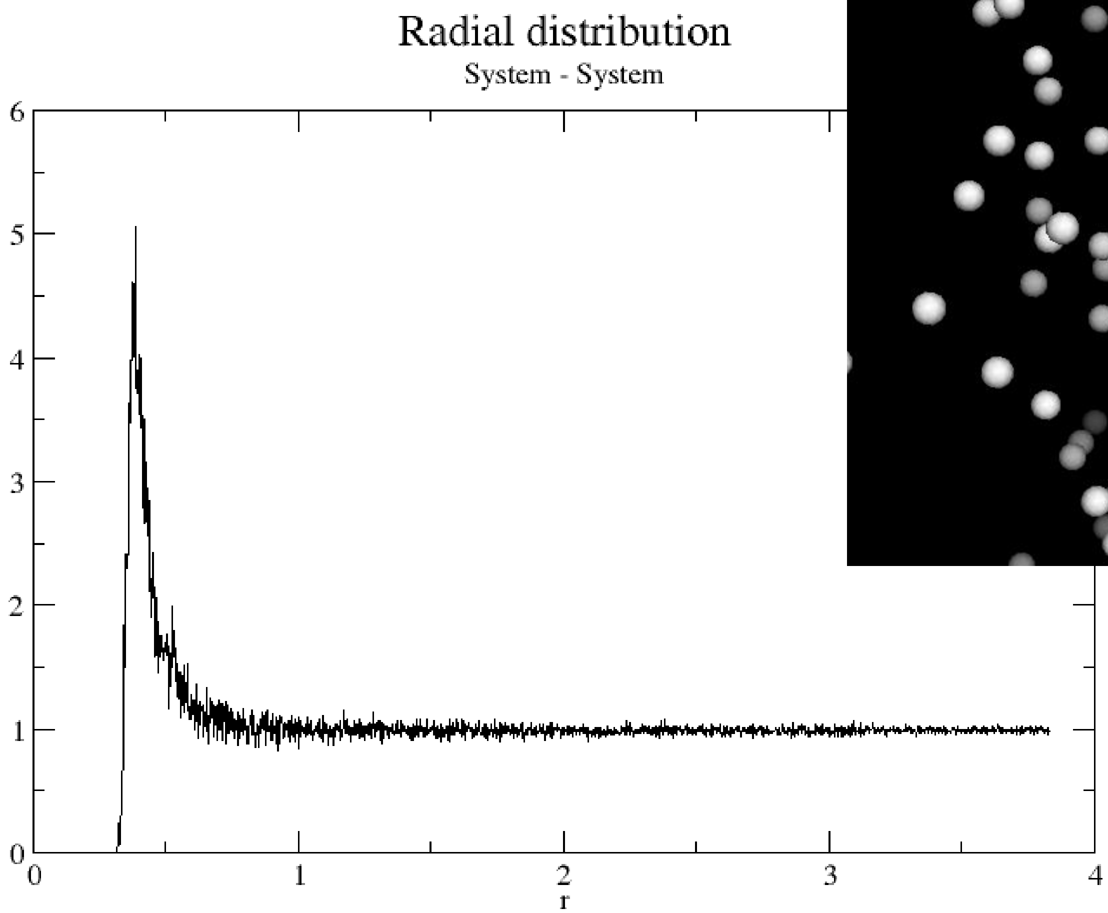
Condensed matter: solids & liquids

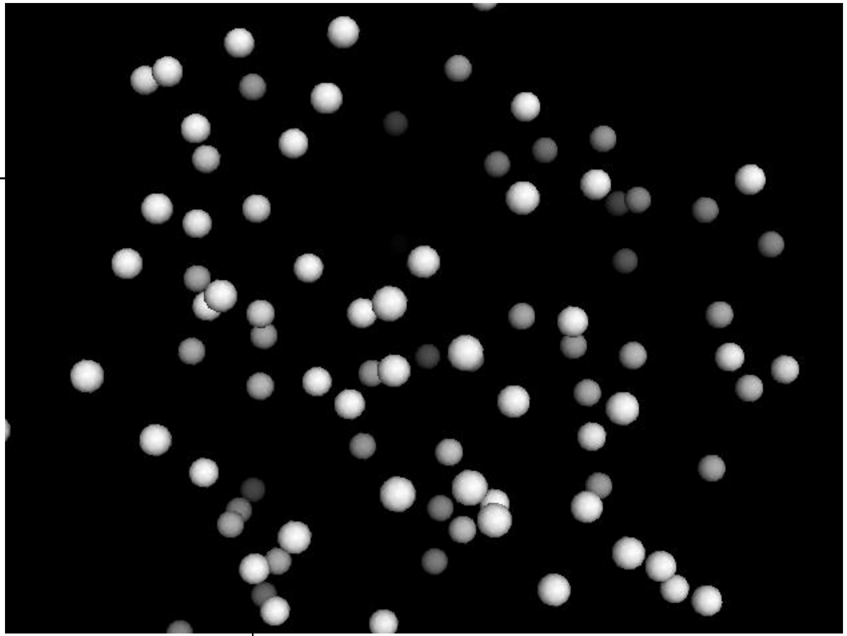
- (Almost) incompressible
- Density changes little with temperature (at constant pressure)

Gases

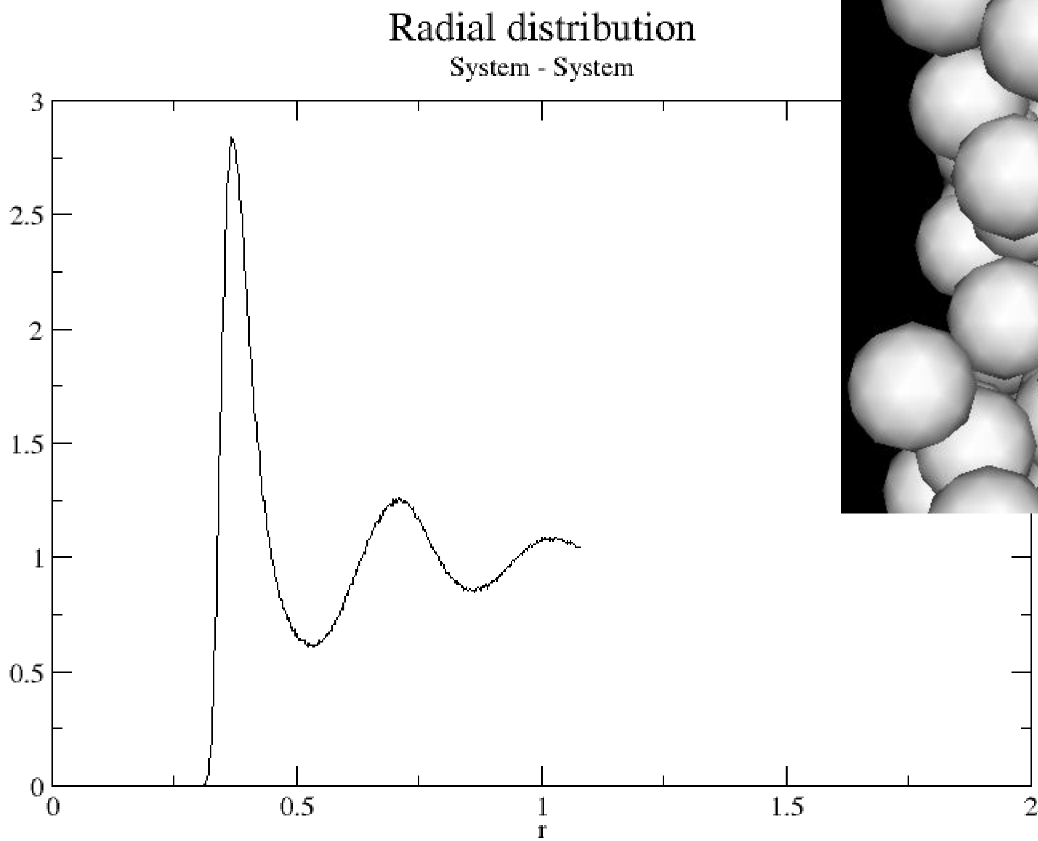
- Easily compressible
- Density changes substantially with temperature (at constant pressure)

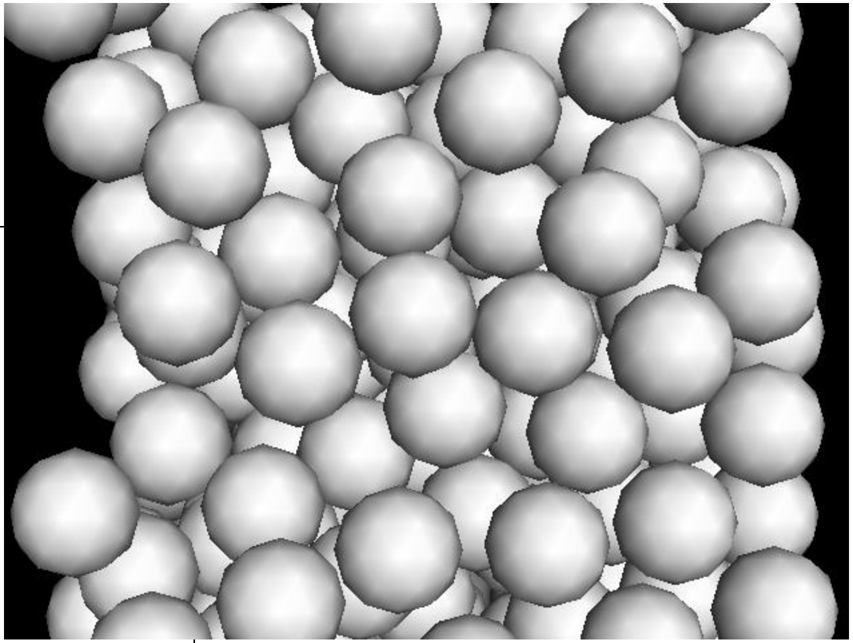
Gases



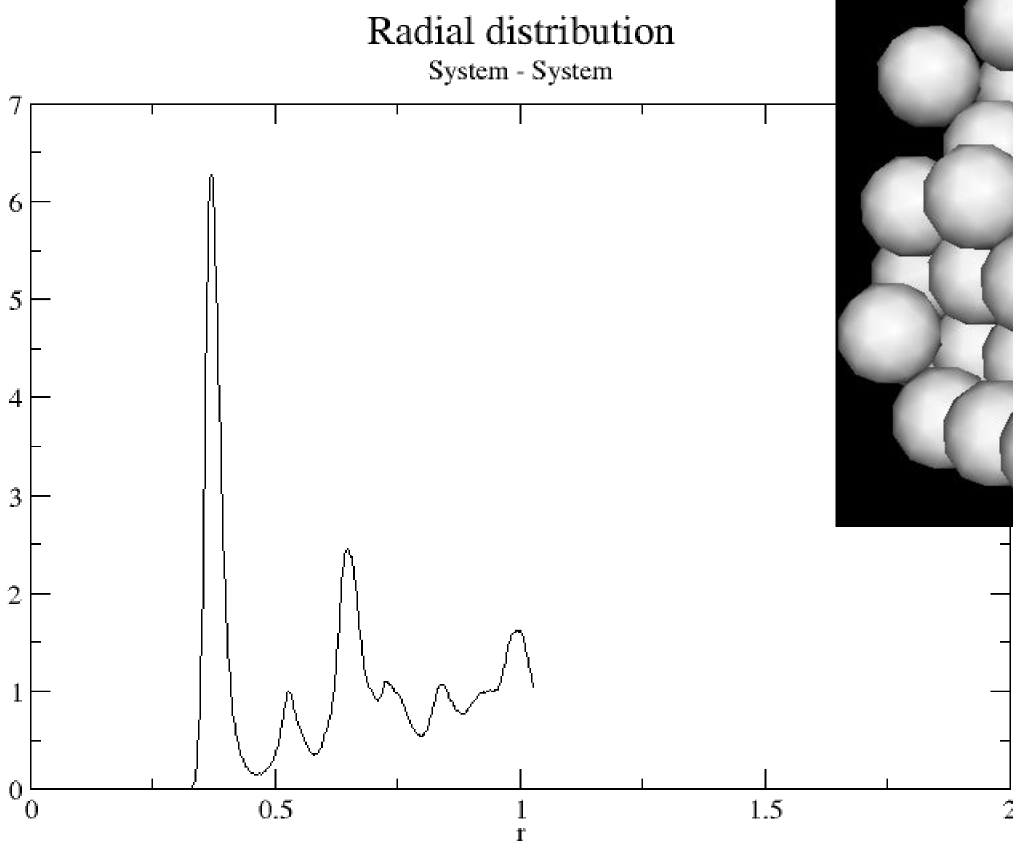


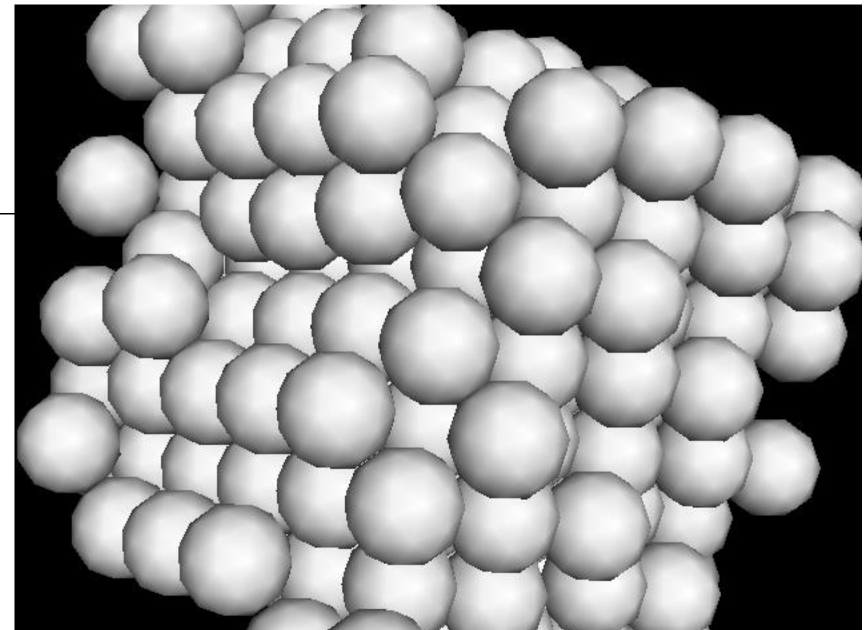
Liquids





Solids





Modern Notions

Gases: full symmetry -- disordered

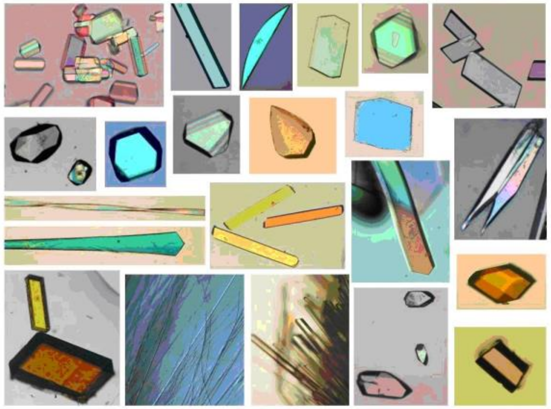
Solids: reduced symmetry -- ordered

- **Think about snowflakes (hexagonal)**

Liquids: short-range order only

Phase transitions

- **Disorder to order: symmetry breaking**
- **Pioneered by Landau, Anderson, …**



Plan

Basic concepts of Thermodynamics

Ideal Gases

The Kinetic Theory of Gases

The First Law of Thermodynamics

The Second Law of Thermodynamics

Entropy and Information