Roundy Research Group

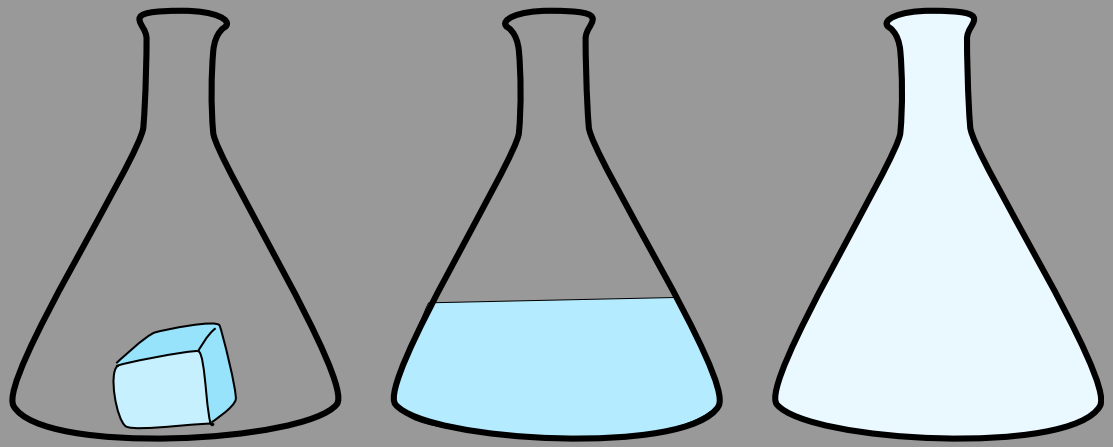
learning about liquids

David Roundy

Oregon State University

What is a liquid?

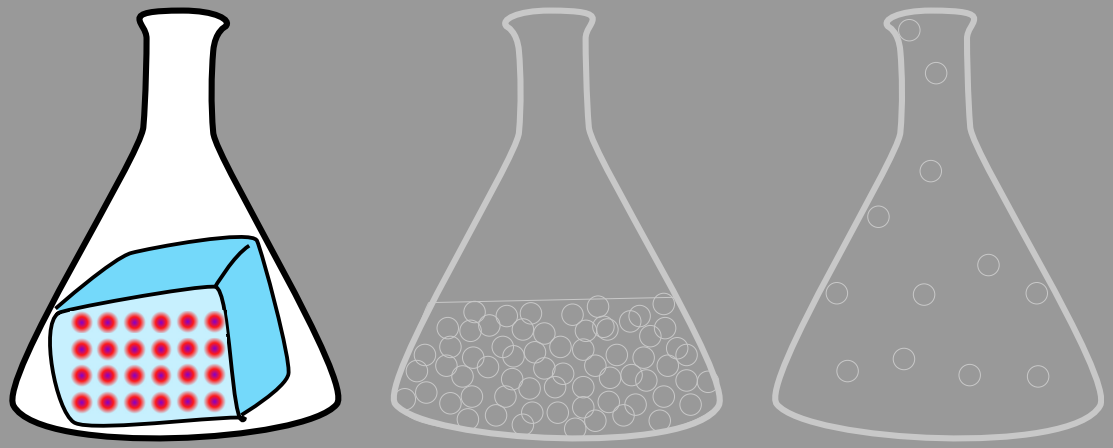
Elementary school definition



Solid	Does not take the shape of its container
Liquid	Takes the shape of a container, but doesn't fill it
Gas	Takes the shape of its container and fills it

What is a liquid?

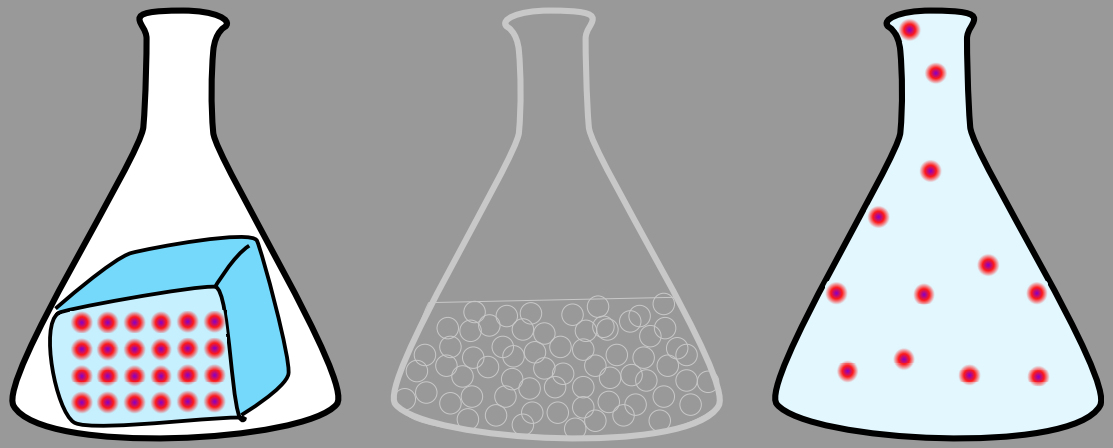
Energy versus entropy



Solid Energy dominates, entropy is a small perturbation

What is a liquid?

Energy versus entropy

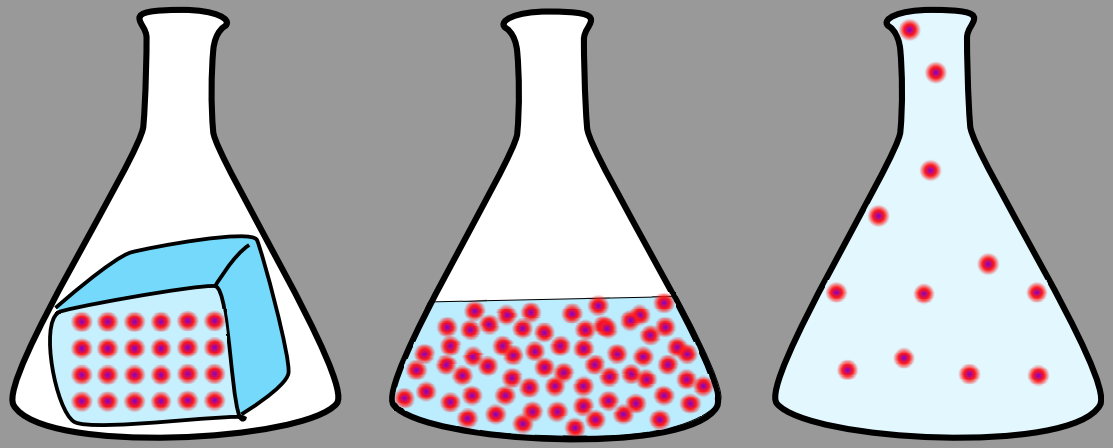


Solid Energy dominates, entropy is a small perturbation

Gas Entropy dominates, energy is a small perturbation

What is a liquid?

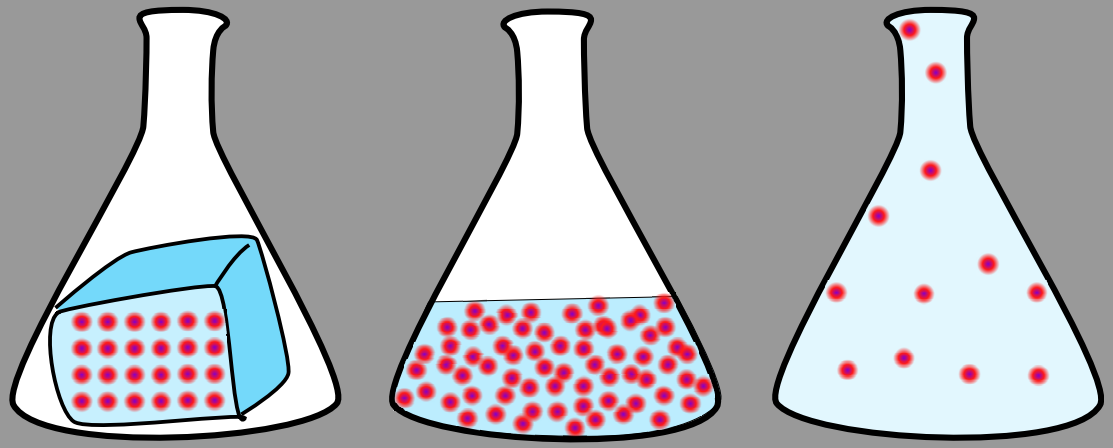
Energy versus entropy



Solid	Energy dominates, entropy is a small perturbation
Liquid	Energy and entropy are balanced
Gas	Entropy dominates, energy is a small perturbation

What is a liquid?

Energy versus entropy



Solid	Energy dominates, entropy is a small perturbation
Liquid	Energy and entropy are balanced
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Perturbation theory

- An "easy" problem we know how to solve
- A "hard" correction that is small
- We construct a power series to solve combined problem

Classical Density Functional Theory

A continuum approach for fluids

Equilibrium density minimizes the Helmholtz free energy

$$\Omega = \min_{n(\mathbf{r})} \left\{ F[n(\mathbf{r})] + \int n(\mathbf{r}) V(\mathbf{r}) d^3 r \right\}$$

where $F[n(\mathbf{r})]$ is a functional describing a fluid, and $V(\mathbf{r})$ is an arbitrary external potential.

Helmholtz free energy

The Helmholtz free energy describes a tradeoff between the energy U and the entropy S.

$$F = U - TS$$

Monte Carlo simulation

Getting the *right* answer for simple models

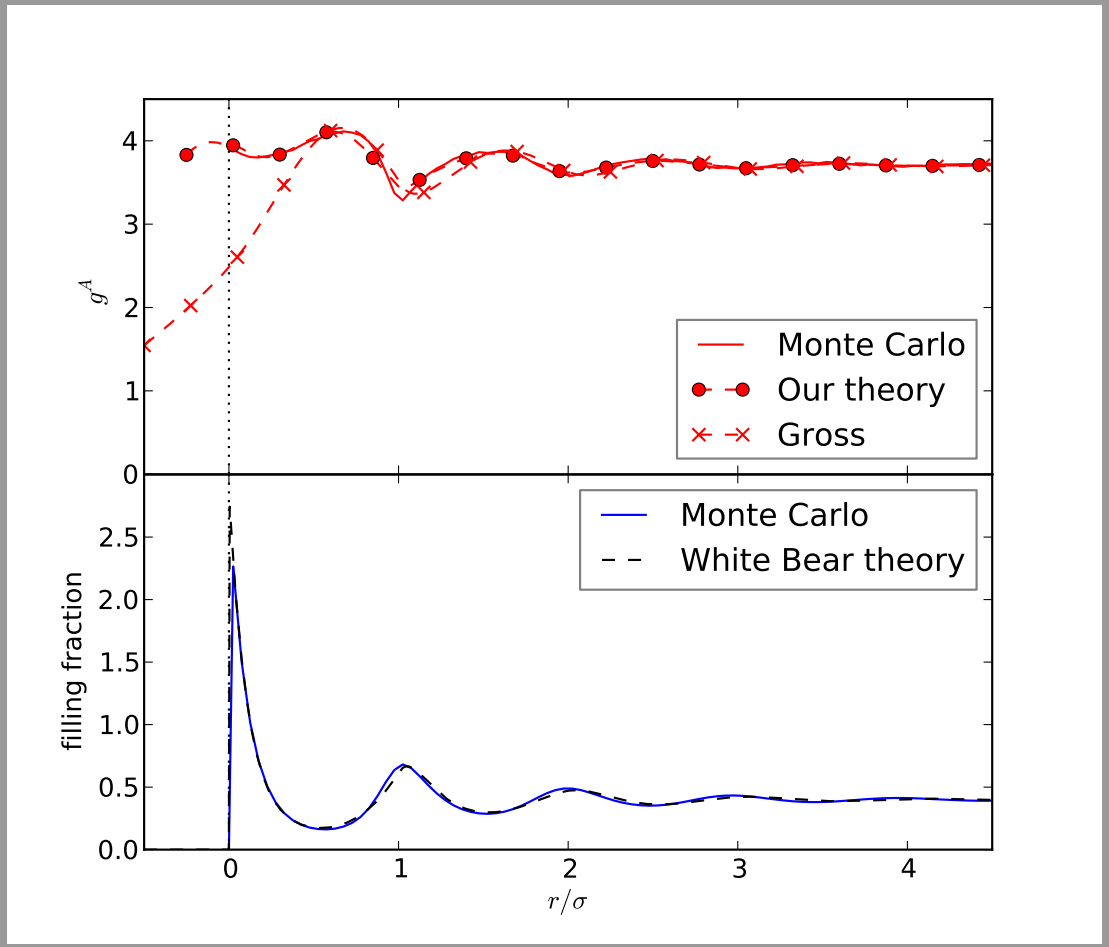
We simulate a number of particles, randomly moving them about subject to appropriate constraints, e.g. they cannot overlap. Using this set of possible configurations

The downside:

- It is *very* slow for large numbers of particles.
- No nice analytical results.

The upside:

- Great for checking the correctness of an analytical theory!


g^A
Monte Carlo
Our theory
Gross
filling fraction
Monte Carlo
White Bear theory
r/σ

Conclusion

Undergraduate students currently in the Roundy Group

1. Chris Haglund
2. Patrick Kreitzberg
3. Rene Zeto
4. Paho Lurie-Gregg
5. Josh Deare

Graduate students currently in the Roundy Group

1. Jeff Schulte
2. Eric Krebs