

# Round Table Discussion

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# Archetypal problem

Define  
Hamiltonian



Simulate it at finite  
temperature

Define free energy  
functional



Minimize it

**Good:** *Mathematicians  
learn from physicists*

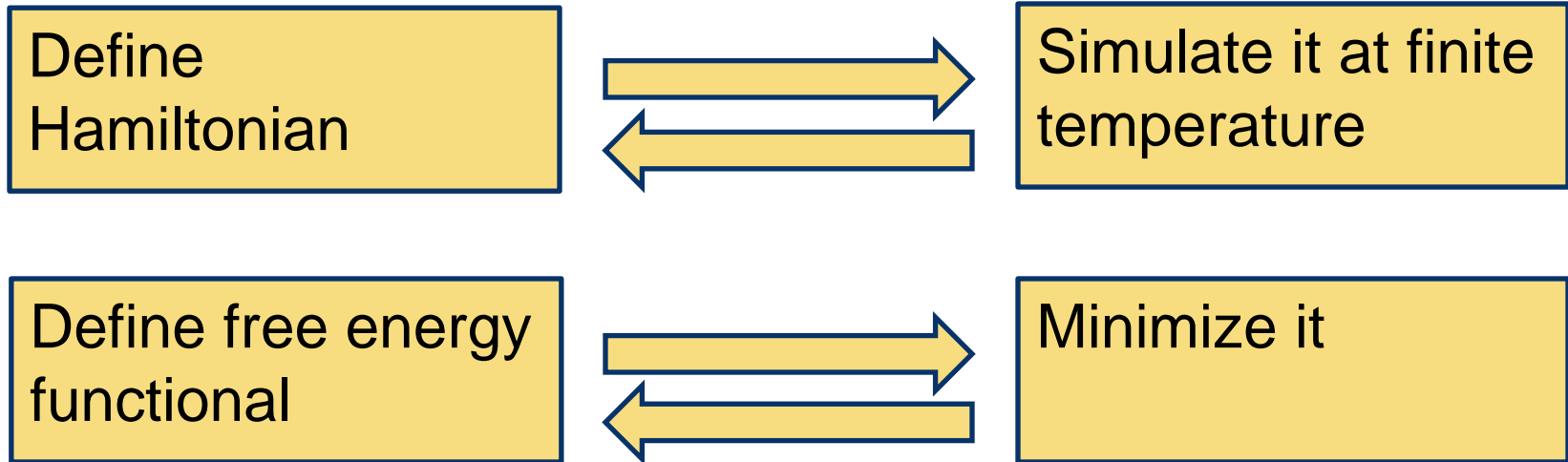
**Better:** *Mathematicians  
and theoretical physicists  
learn from experimental  
physicists and chemists*

**Methods:**

*Monte Carlo  
Molecular dynamics*

*PDE algorithms  
Finite element*

# Discussion point #1



## ***Lemma:***

*If minimizing your free energy gives you crazy results, then you are minimizing the wrong free energy.*

Two methods are missing from the list.  
What happened to them?

1. Construct variational ansatz, insert into free energy, minimize over parameters.
2. Don't just minimize over order parameters; ***integrate*** over order parameters to account for thermal fluctuations.

## Polydispersity as an axis in a phase diagram

- Methods to treat polydispersity
  - Know how to describe systems with 2 components (or a small number of components)  
⇒ 2-phase coexistence regions in phase diagram
  - Does new behavior emerge when there are many components?
- Effects of polydispersity
  - On crystalline or smectic order
  - On orientational order

Among all the topics discussed in this workshop, we have seen a strong emphasis on modeling biaxial nematic phase.

- Why?
  - Experimental controversy?
  - Technological applications?
- Principles that can be applied to other types of order?
  - Polar
  - Generalized nematic: Cubatic, tetrahedratric
  - Quasicrystalline