Introduction

What is thermo & kinetics

Thermodynamics
Energy, Entropy, Temperature
"do work"?

"Laws" are empirical
& Equilibrium

Kinetics

① motion of atoms

② reaction rates

∴ relax to equilibrium

Statistical thermodynamics

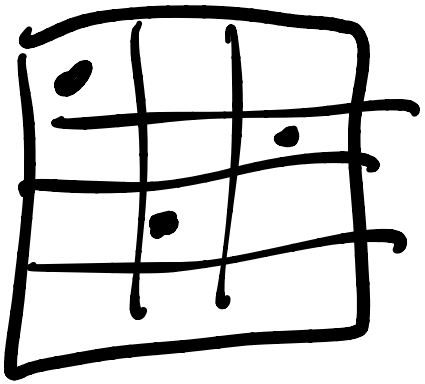
Late 1800 → now

molecular interactions → properties

Modern times

- small systems "violate" laws of thermodynamics
  "fluctuations"

simple models → unifying concepts



ideal gas

$\in$ # bound proteins by a drug

↖ # sites catalyst bound reactant

Mathematics & Statistics

Language of thermodynamics

Calculus:

change / flow of heat

change in entropy ...

Work done in a process

→ area under curve

Statistics → probabilities, avg, variance

- experimental data

Data & Programming

- fitting real data
- simulate to test hypotheses
  model → data
- AI models → code → simulate

What isn't thermodynamics

Quantum mechanics

→ systems have discrete states

Current problems

① Health & medicine

how do we design drugs?

how do proteins fold

② predict structure of proteins RNA ... (Nobel Prize 2024)

③ Machine learning

④ Sustainability