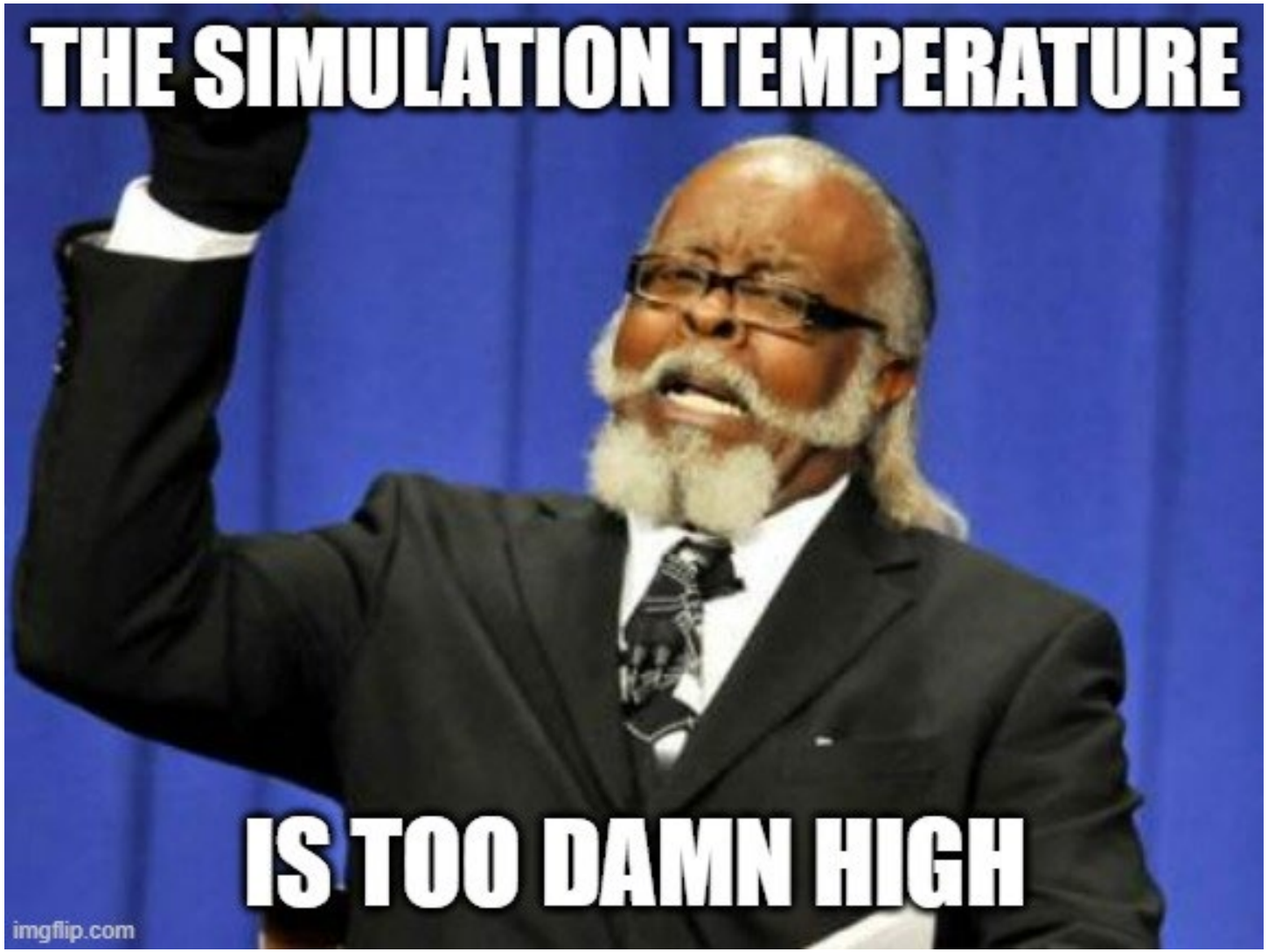
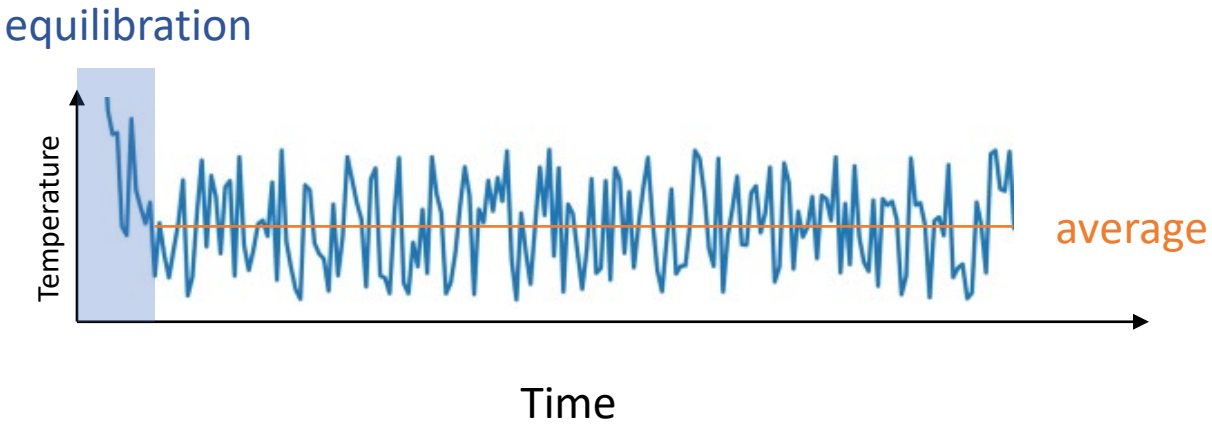
MD /MC



Temperature

Instantaneous vs. average temperature



How to best choose starting velocities if we want to simulate at temperature T?

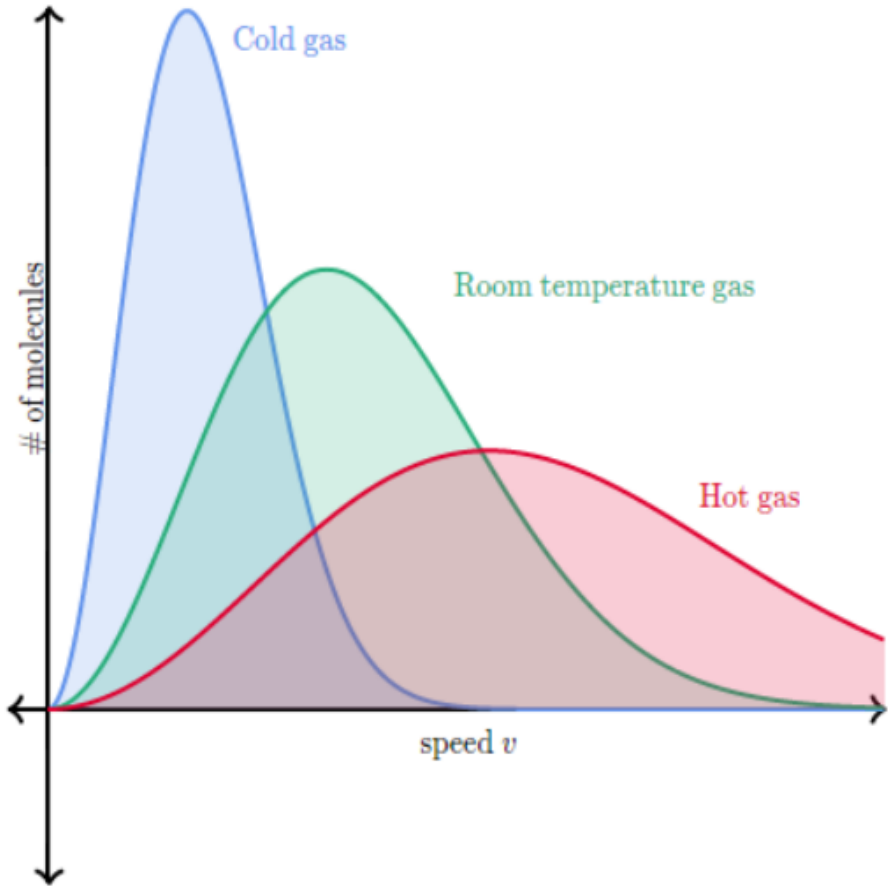


Fig. 5.5 Maxwell Boltzmann distribution for three different temperatures. Figure CC by SA Khan Academy

How to sample in NVT?

MC

Easy

Accept moves according to Boltzmann distribution at target temperature

MD

Tricky, we need to couple our system to a heat bath to exchange heat to stay at correct temperature, by default NVE

Many methods: Global or Local

Global Thermostat

Compute temperature at each step and make all particles slower/faster if they do not match target temperature

- At each step: Velocity rescale
- With lag over a few steps: Berendsen

Advanced: Extra degree of freedom e.g Nose Hoover

Local Thermostat

random collisions to change individual particles

Andersen thermostat: Particles randomly get assigned a new velocity from the Maxwell Boltzmann distribution

Can we sample correct physical dynamics in NVT?

Flying ice cube

Equipartition is important

With Berendsen we might drain all energy from high-frequency modes (vibrations) in low-frequency modes such as translation. Our system still has our target average temperature but equipartition is violated.


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Table 1. Basic summary of popular thermostats. ✗ indicates that the thermostat does not fulfill the statement, ✓ indicates that the thermostat does fulfill the statement, and (✓) indicates that the thermostat fulfills the statement under certain circumstances.

Thermostat	Ensemble	Deterministic/ Stochastic	Global/ Local	Physical?	Correct Structural Properties?	Correct Dynamical Properties?
None	Microcanonical	Deterministic		✓	✓	✓
Gaussian	Isokinetic	Deterministic	Global	✗	✓	✗
Simple Velocity Rescaling	Undefined	Deterministic	Global	✗	✗	✗
Berendsen	Undefined	Deterministic	Global	✗	✗	✗
Bussi	Canonical	Stochastic	Global	✗	✓	(✓)
Andersen	Canonical	Stochastic	Local	✗	✓	✗
Langevin	Canonical	Stochastic	Local	✗	✓	✗
Nosé-Hoover	Canonical	Deterministic	Global	✗	✓	(✓)

Best practices for MD simulations:
https://livecomsjournal.org/index.php/livecoms/article/view/v1i1e5957