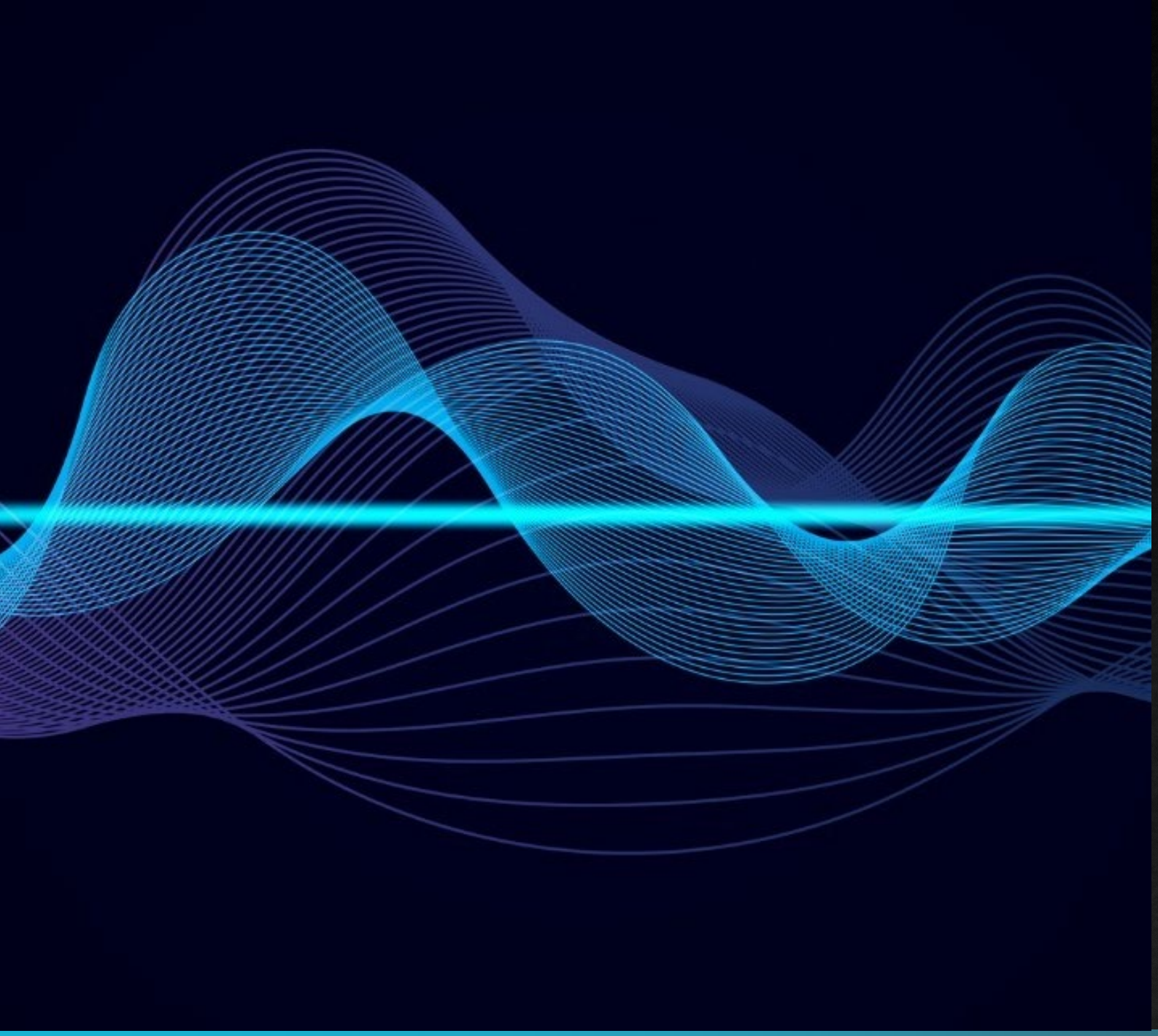


Computational Physics

PHYS 6260

Monte Carlo Simulations

Announcements:

- HW4: Due Friday 2/7
- HW5: Due Friday 2/14
- Traveling next week. Will post recorded lectures on Teams.

Lecture Outline

We will cover these topics

- Application: Cosmology and large-scale structure
- Importance sampling and statistical mechanics
- Markov Chain method

Introduction

- All branches use Monte Carlo (MC) simulations
- Models physical processes with random numbers
- The largest user of MC simulations is statistical mechanics
- Statistical mechanics is fundamentally the description of apparently random processes

- Before looking at statistical mechanics, let's inspect how cosmological simulations (my expertise) are performed with dark matter

Application overview: Cosmology

- QM fluctuations seed all large-scale structure at $t < 10^{-20}$ seconds after Big Bang
- These density fluctuations grow in size with the Universe's expansion
- After some time, they start to gravitationally collapse

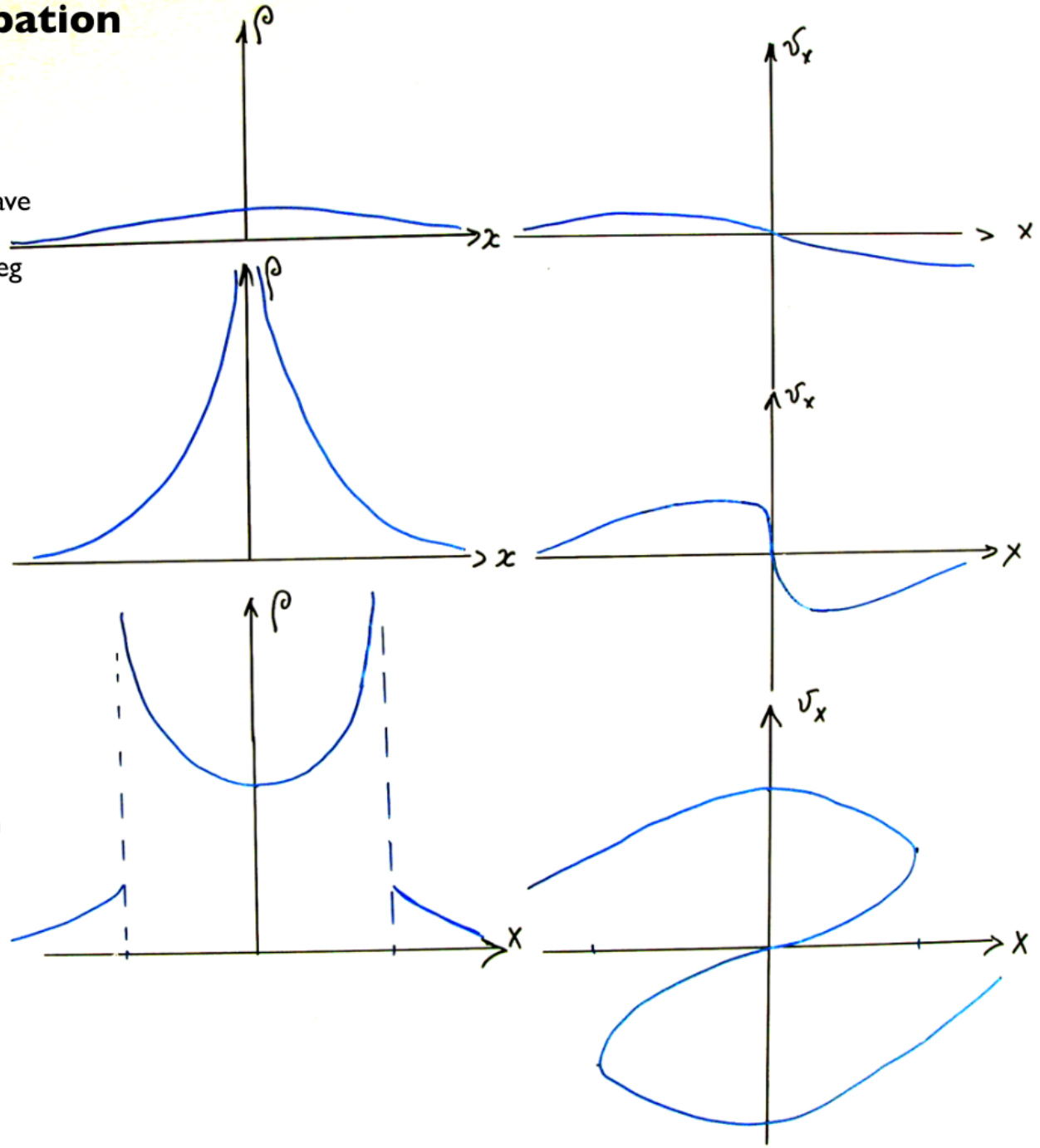
- Dark matter makes up ~5/6 of all matter and is thought to be composed of an unknown particle
- Treated like a collisionless fluid (think of dust)
- It has some continuous distribution function, but we coarsely sample it with massive particles
- Let's look at the 1D case (Zel'dovich approximation)

Evolution of a 1D perturbation

Early stages of evolution: small-amplitude wave produces an overdensity around x= 0. Perturbation in velocity goes in phase (90 deg difference) with the density perturbation

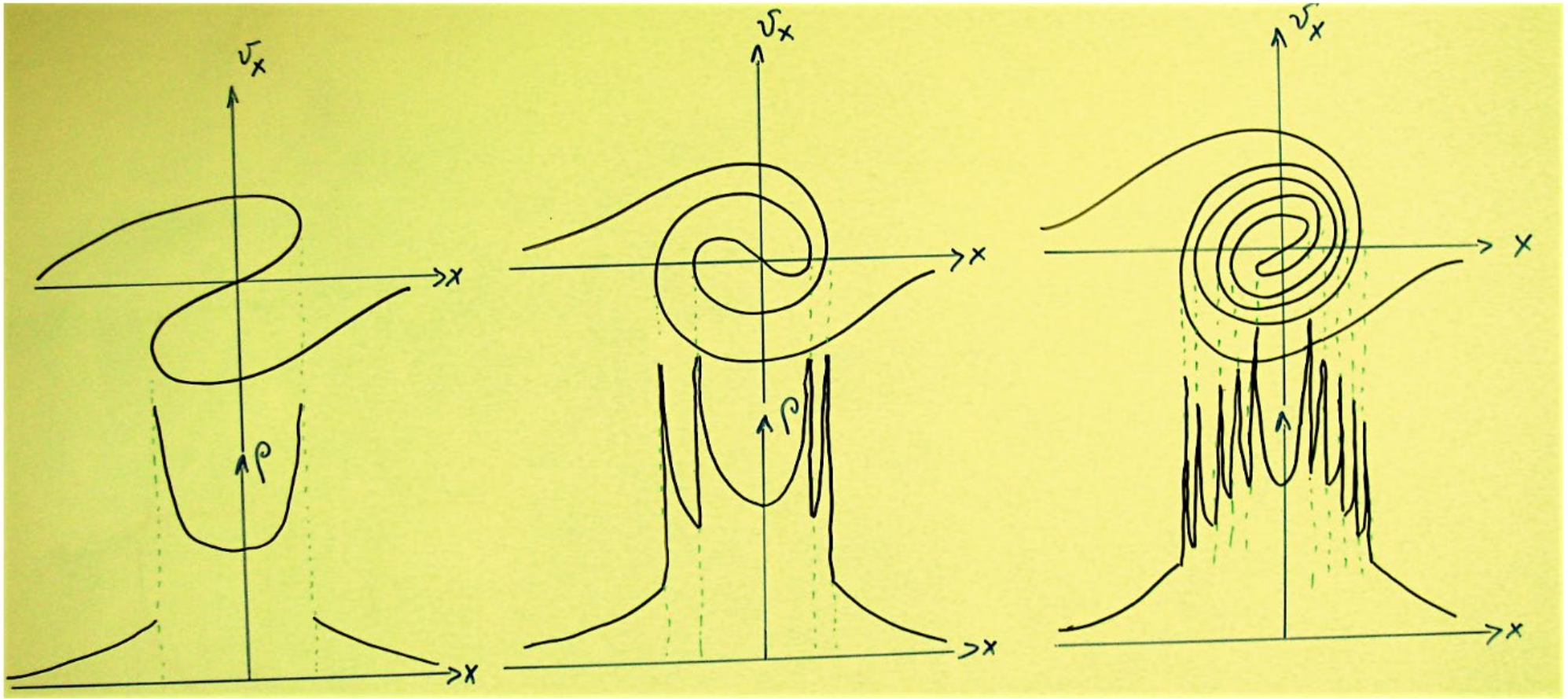
Formation of caustic: density is infinite at x=0. The curve of V(x) has vertical slope at the same x=0 distance.

At later stages particles still keep moving along their initial direction: they do not turn around in the Zeldovich approximation. Now we have two caustics, which move away from the central x=0 plane. At each point inside the region of the caustics there are three flows.

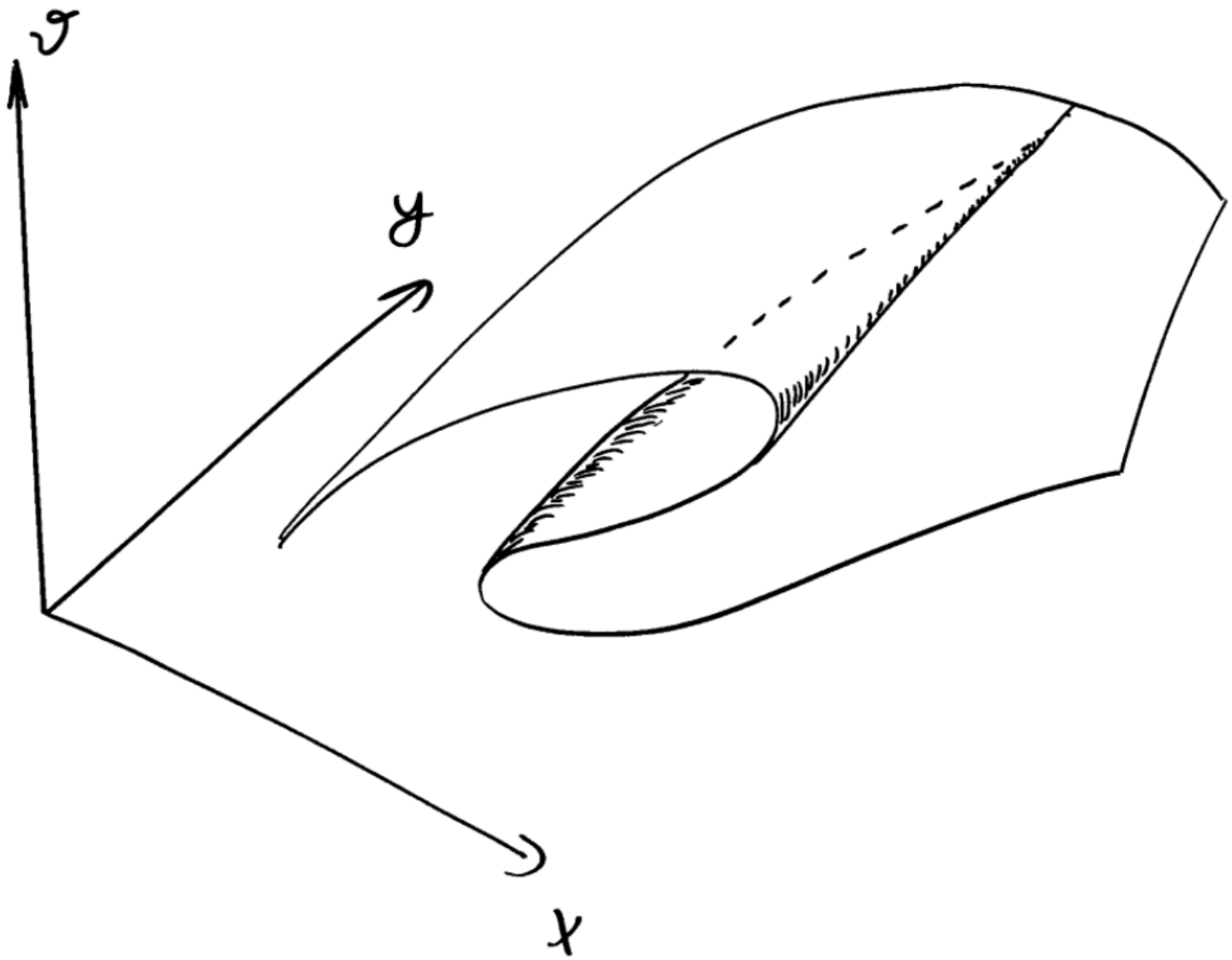


Evolution of a 1D perturbation: beyond Zeldovich approximation

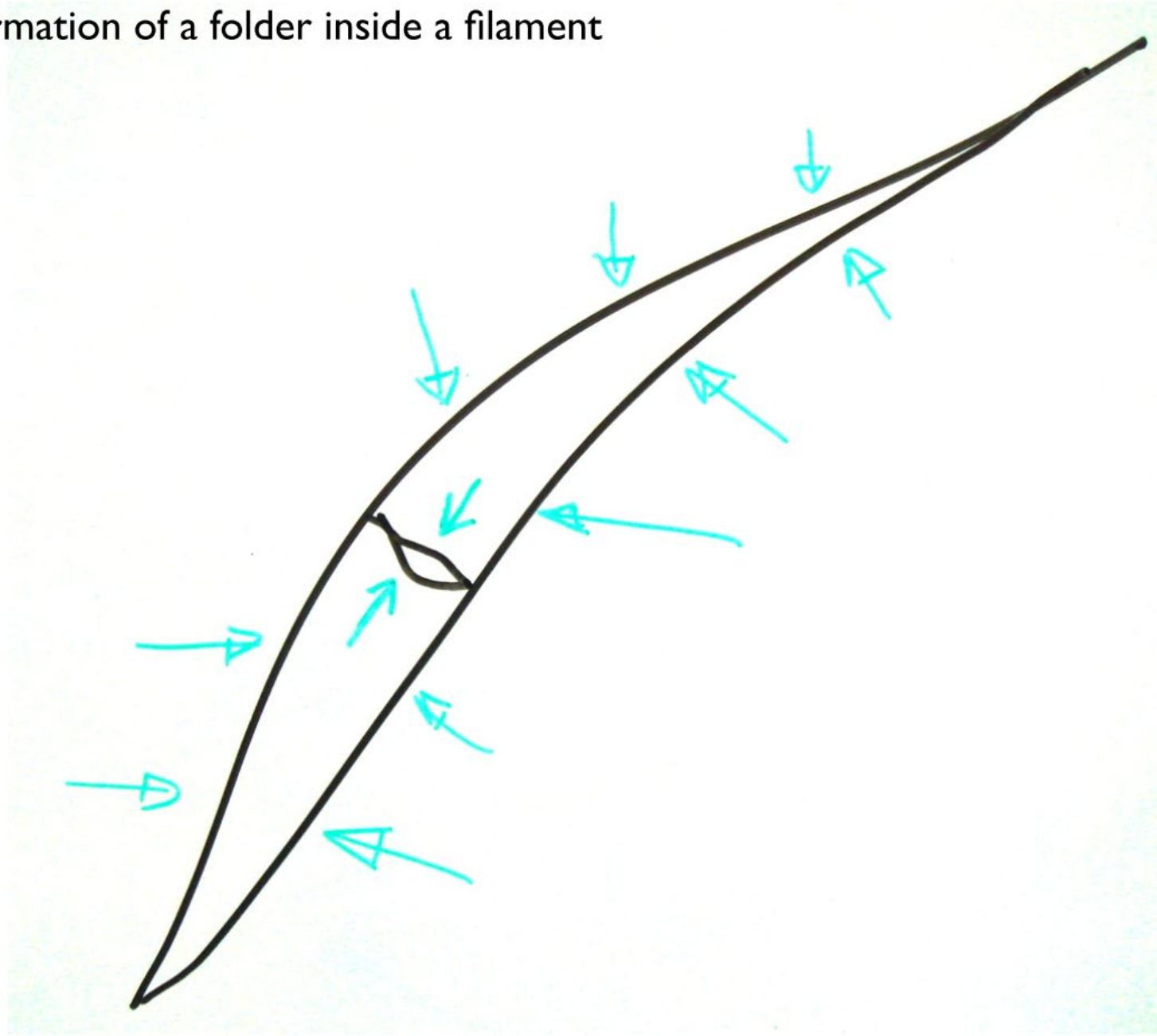
In reality, particles will move away from the center for a short while, then turn around and fall back. This produces a more complicated picture illustrated below. Each folder in the velocity space produces two caustics in real space. At each point in real space there are odd number of flows: 1,3, 5...



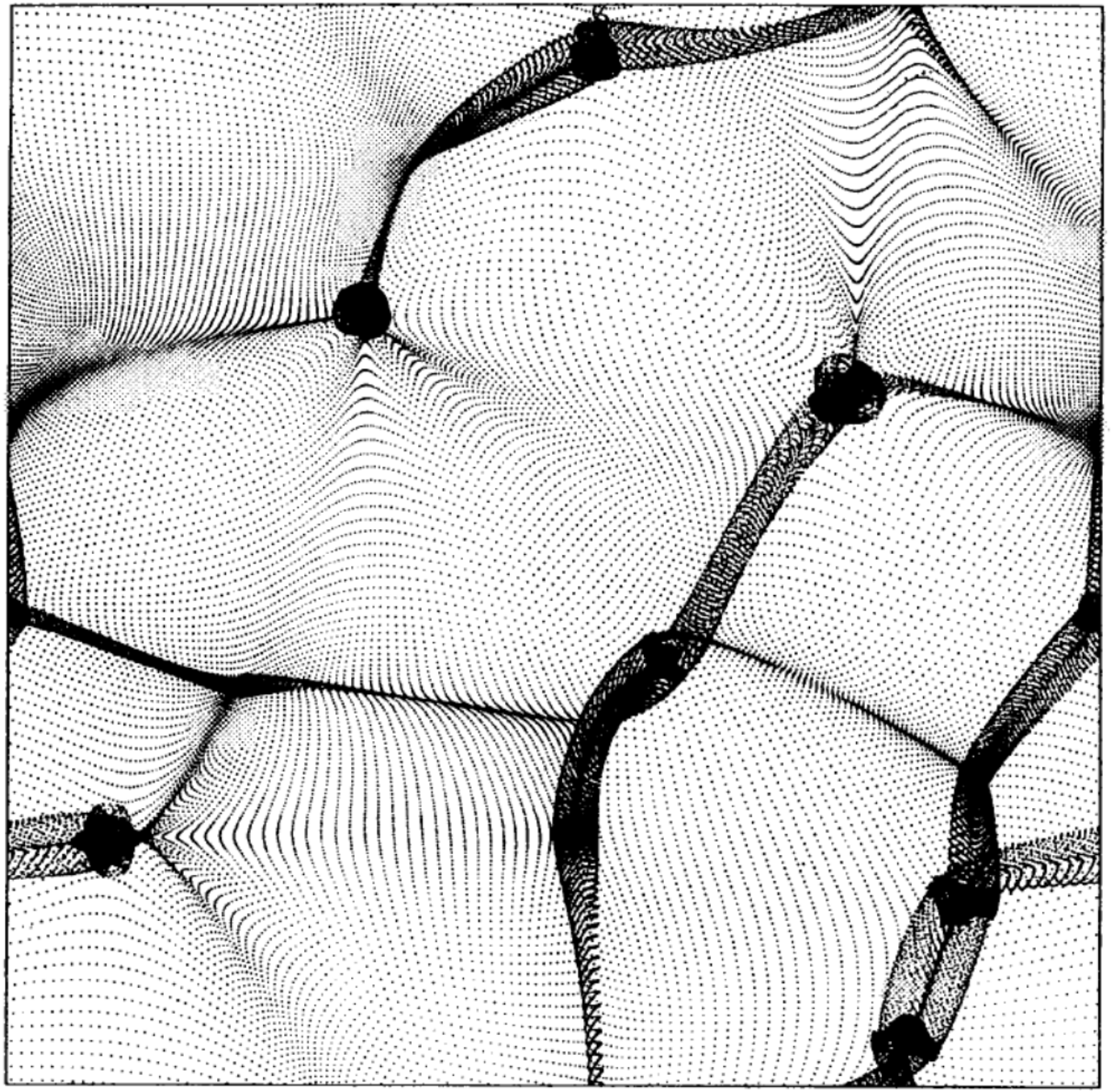
In 2 dimensions:



In 2 dimensions: formation of a folder inside a filament

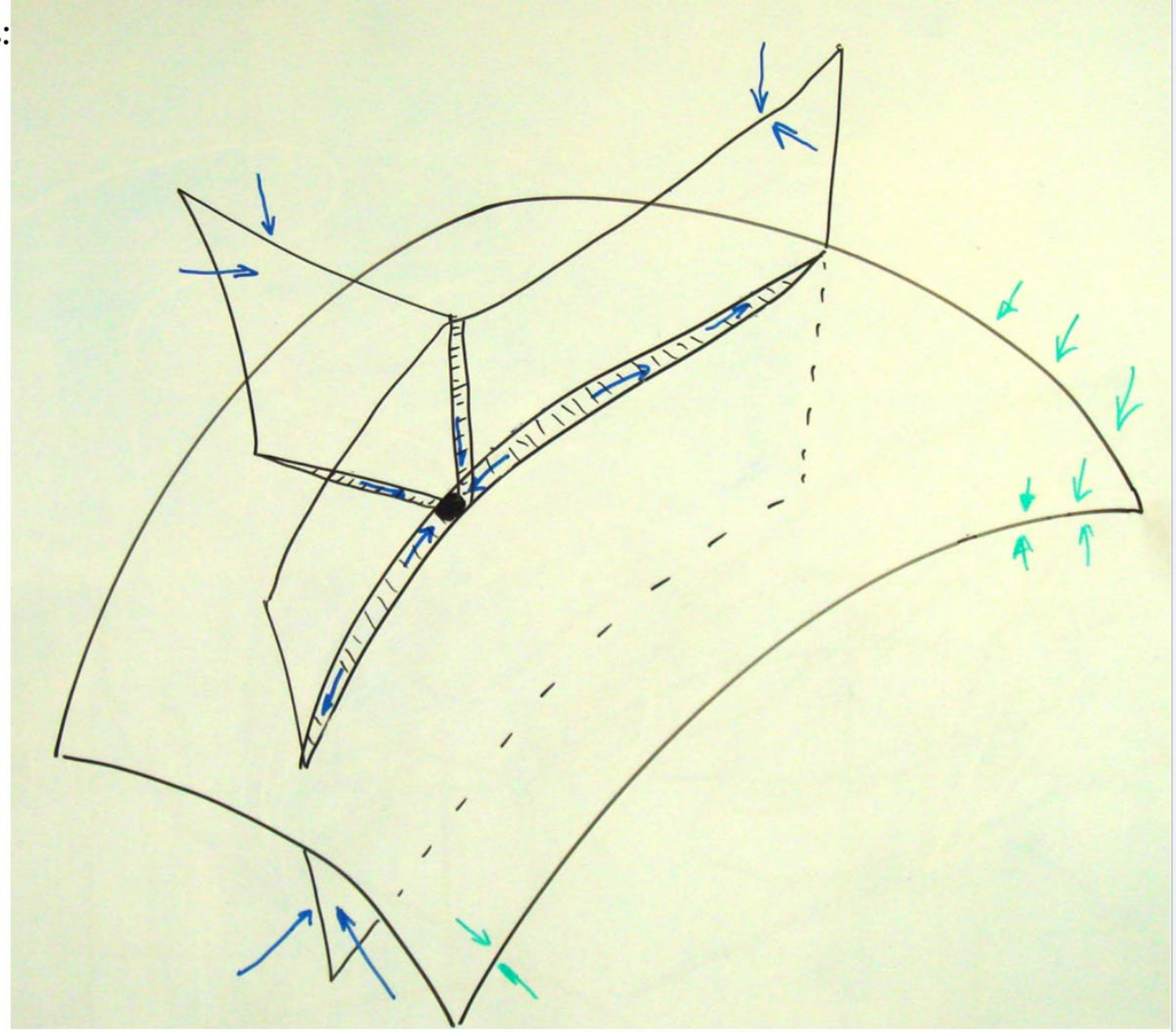


Formation of caustics in a simplified 2D model, which has only very few long-wave harmonics



Sahni et al 1994

3 dimensions:



Large scale structure: 326M light-years across: 13 Gyr of evolution

Importance sampling: Stat mech

- Consider a system with temperature T
- Fundamental stat mech problem: calculating average value of a quantity
- Stat mech describes the system to have some probability of occupying some state i with energy E_i, given by the Boltzmann formula and partition function Z

$$P(E_i) = \frac{e^{-\beta E_i}}{Z}, \qquad Z = \sum_i e^{-\beta E_i}, \qquad \beta = \frac{1}{k_B T}$$

- The average quantity Z has a value X_i in the i^{th} state

$$\langle X \rangle = \sum_i X_i P(E_i)$$

- We can't sum over all the states because there are too many of them

Importance sampling: Stat mech

$$P(E_i) = \frac{e^{-\beta E_i}}{Z}, Z = \sum_i e^{-\beta E_i}, \beta = \frac{1}{k_B T}$$

- We can use importance sampling to integrate over this essentially infinite domain
- Choose N states (each state k) at random and take the average value over them

$$\langle X \rangle \simeq \frac{\sum_{k=1}^{N} X_k P(E_k)}{\sum_{k=1}^{N} P(E_k)}$$

- There are many states with $E_i \gg k_B T$ that contribute very little to the average
- There is a range of states that contribute the most to the average
- We want to use important sampling to favor choosing these states

Importance sampling: Stat mech

$$\langle X \rangle \simeq \frac{\sum_{k=1}^{N} X_k P(E_k)}{\sum_{k=1}^{N} P(E_k)}$$

- We will take a weighted average (weight is unknown)

$$\langle g \rangle_w = \frac{\sum_i w_i g_i}{\sum_i w_i}$$

- Let's inspect the function $g_i = X_i P(E_i)/w_i$

$$\left\langle \frac{X_i P(E_i)}{w_i} \right\rangle_w = \frac{\sum_i w_i X_i P(E_i)/w_i}{\sum_i w_i} = \frac{\sum_i X_i P(E_i)}{\sum_i w_i} = \frac{\langle X \rangle}{\sum_i w_i}$$

- Solving for $\langle X \rangle$

$$\langle X \rangle = \left\langle \frac{X_i P(E_i)}{w_i} \right\rangle_w \sum_i w_i$$

Importance sampling: Stat mech

$$\langle X \rangle = \left\langle \frac{X_i P(E_i)}{w_i} \right\rangle_w \sum_i w_i$$

- But what do we use as a weighting function?
- To choose a random state that favors the most probable states, we can simply use the probability function $P(E_i)$
- Recall that $P(E_i)$ is normalized, $\sum_i w_i = 1$
- Now the weighted average is

$$\langle X \rangle \simeq \frac{1}{N} \sum_{k=1}^{N} X_k,$$

- The k states are chosen from the Boltzmann formula's probability, $e^{-\beta E_i}$

Markov Chain method

- Choosing a random state isn't enough to fully describe the system
- The partition function Z is the sum over all states
- Cannot address Z on a 1-to-1 basis
- However, we can choose random states without knowing Z using a Markov Chain

- Start with some state i. Choose the next state j that is connected to i
- This is a move set that changes the system by one degree of freedom

Markov Chain method

- Consider a set of N molecules, each with its own quantum state
- A move set would change the state of one molecule only
- The change to a new state is determined by a set of transition probabilities T_{ij}
- If T_{ij} is chosen right, the Boltzmann probability $P(E_i)$ will be recovered given enough changes
- The transition probabilities are inherently normalized, $\sum_j T_{ij} = 1$
- The key in this method is make the partition function vanish

$$\frac{T_{ij}}{T_{ji}} = \frac{P(E_j)}{P(E_i)} = \frac{e^{-\beta E_j}/Z}{e^{-\beta E_i}/Z} = e^{-\beta(E_j - E_i)}$$

Markov Chain method

- What if we achieve a perfect solution during the chain?
- Inspect the probability of choosing state j on the next step
- It's the sum of the probabilities along the chain with every other possible state i

$$\sum_i T_{ij} P(E_i) = \sum_i T_{ji} P(E_j) = P(E_j) \sum_i T_{ji} = P(E_j),$$

- Proves that once a Markov chain obtains the Boltzmann probability, it will remain there indefinitely
- Also the Markov chain will converge given enough changes
- But what is T_{ij} that controls the move sets?

Markov Chain method

$$\sum_i T_{ij} P(E_i) = \sum_i T_{ji} P(E_j) = P(E_j) \sum_i T_{ji} = P(E_j),$$

- The move set can be chosen at random (uniformly) but doesn't satisfy the equation above
- The Metropolis algorithm determines whether or not to accept the change with a probability of

$$P_a = \begin{cases} 1 & \text{if } E_j \leq E_i \\ e^{-\beta(E_j - E_i)} & \text{if } E_j > E_i \end{cases}$$

- If the total energy of the system decreases, we accept the change
- If the total energy of the system increases, there's some non-zero probability we accept it

Summary: Markov Chain method

1. Choose a random initial state
2. Choose a move uniformly at random from an allowed set of moves
3. Calculate the value of the acceptance probability P_a
4. Accept or reject the proposed change
5. Measure the value of the quantity X in the current state and add it to a running sum of such measurements
6. Repeat from step 2

Subtleties: Markov Chain method

- When a move is rejected, the quantity X must still be measured and added to the sum
- When choosing a new state, every possible state must be accessible through some path. This is known as an ergodic move set
- Although we know that a Markov chain will converge toward the answer, it's unknown exactly how long it will take to equilibrate

MC Simulation of an Ideal Gas

In-class problem

- The QM states of a particle/atom of mass m in a cubic box of length L have three integer quantum numbers $(n_x, n_y, n_z) = 1 \ \ldots \infty$ with energies of

$$E(n_x, n_y, n_z) = \frac{\pi^2 \hbar^2}{2mL^2} (n_x^2 + n_y^2 + n_z^2)$$

- The total energy is the sum of individual particle energies
- Consider a move set where one of the quantum numbers is randomly changed by ± 1
- The corresponding change in energy is

$$\Delta E = \frac{\pi^2 \hbar^2}{2mL^2} (\pm 2n_i + 1)$$

MC Simulation of an Ideal Gas

In-class problem

$$P_a = \begin{cases} 1 & \text{if } E_j \leq E_i \\ e^{-\beta(E_j - E_i)} & \text{if } E_j > E_i \end{cases}$$

- Simulate an ideal gas with N = 1000 particles
- Start with the "ground state" of $n_x = n_y = n_z = 1$
- The system has a temperature of $k_B T = 10$
- For simplicity, set $\hbar = m = L = 1$
- Don't allow the quantum numbers to drop below 1
- Execute the Markov chain 250,000 times

$$E(n_x, n_y, n_z) = \frac{\pi^2 \hbar^2}{2mL^2}(n_x^2 + n_y^2 + n_z^2)$$

$$\Delta E = \frac{\pi^2 \hbar^2}{2mL^2}(\pm 2n_i + 1)$$

- Plot how the total energy changes with each iteration
- Plot the distribution of final state of quantum numbers