PHY604 Lecture 21

November 6, 2025

Today's lecture:
Monte Carlo integration and simulation

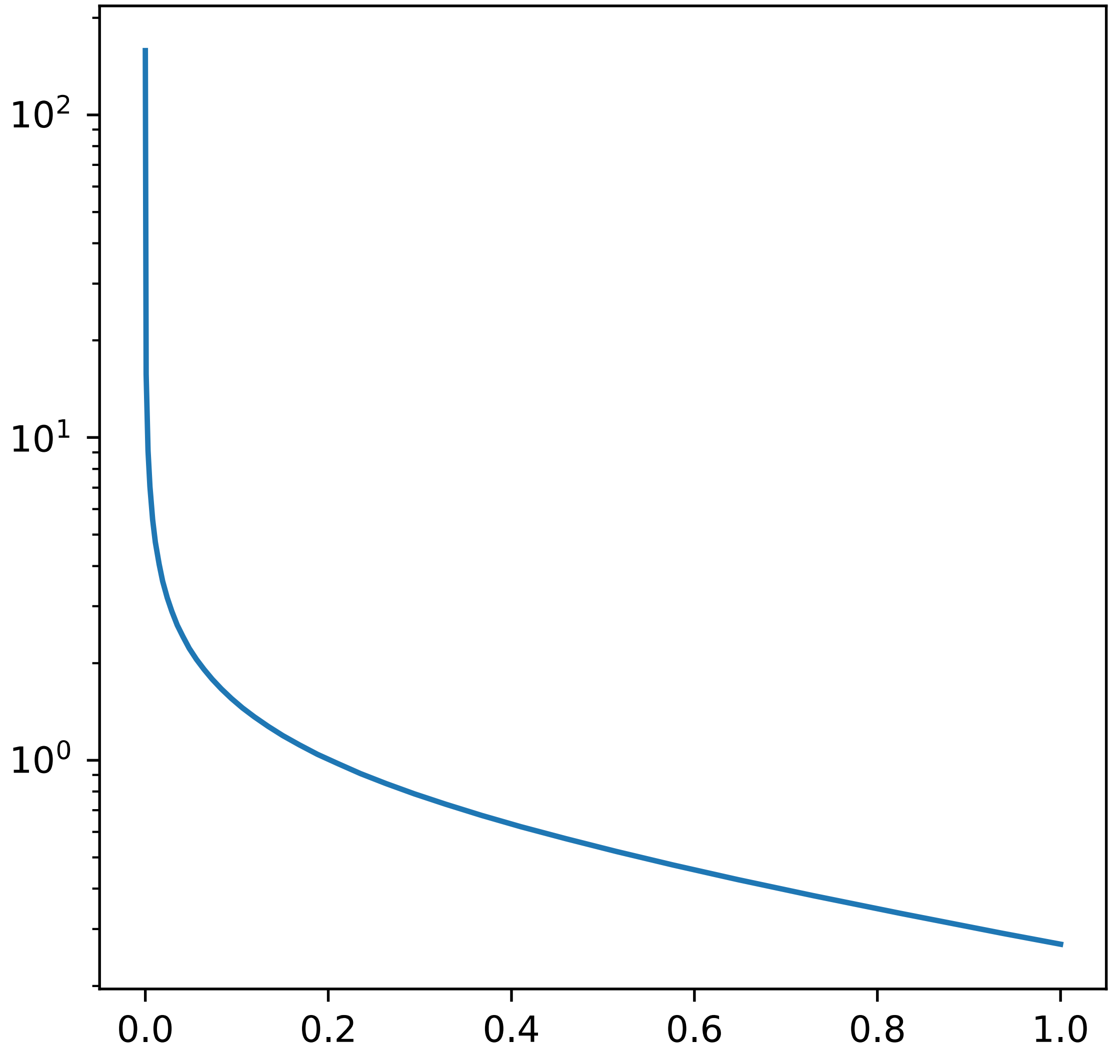
- Monte Carlo integration with divergences
- Monte Carlo simulation

Monte Carlo integration with divergences

- Monte Carlo integration fails for some pathological functions, e.g., those that contain divergences
- Consider:

$$I = \int_0^1 \frac{x^{-1/2}}{e^x + 1} dx$$

- Function diverges at *x*=0, but integral is finite
- E.g., for mean value method, will occasionally get a very large contribution
  - Estimate varies widely between runs



Importance sampling

- Can get around these issues by drawing points nonuniformly
- For a general function *g*(*x*) can define a weighted average:

$$\langle g \rangle_w = \frac{\int_a^b w(x) g(x) dx}{\int_a^b w(x) dx}$$

- *w*(*x*) is a weighting function
- If we want to solve a general 1D integral: $I = \int_a^b f(x) dx$
- We set *g*(*x*)=*f*(*x*)/*w*(*x*):

$$\left\langle \frac{f(x)}{w(x)} \right\rangle_w = \frac{\int_a^b f(x) dx}{\int_a^b w(x) dx} = \frac{I}{\int_a^b w(x) dx}$$

Importance sampling, 1D integral

- Thus, we have:

$$I = \left\langle \frac{f(x)}{w(x)} \right\rangle_w \int_a^b w(x)dx$$

- Equivalent to the mean value method, but from a weighted average

- How do we calculate the weighted average?

- Define probability density function as normalized *w*(*x*)

$$p(x) = \frac{w(x)}{\int_a^b w(x)dx}$$

- So

$$\langle g \rangle_w = \int_a^b p(x)g(x)dx$$

Importance sampling, 1D integral

- Now let's sample *N* random points in the interval with the distribution *p*(x). Then:

$$\sum_{i=1}^{N} g(x_i) \simeq \int_a^b Np(x)g(x)dx$$

- So:

$$\langle g \rangle_w = \int_a^b p(x)g(x)dx \simeq \frac{1}{N}\sum_{i=1}^{N} g(x_i)$$

- Where x_i are chosen from the distribution:

$$p(x) = \frac{w(x)}{\int_a^b w(x)dx}$$

Importance sampling, 1D integral

- Putting everything together:

$$I \simeq \frac{1}{N}\sum_{i=1}^{N}\frac{f(x_i)}{w(x_i)}\int_a^b w(x)dx$$

- Generalization of mean value method, which is where *w*(*x*)=1
- *w*(*x*) can be any function that we choose
  - Can be chosen to remove pathologies in the integrand
- However, now we need to draw from a nonuniform distribution

Error on importance sampling method

- Error is given by:

$$I_{\text{error}} = \frac{\sqrt{\text{var}_w(f/w)}}{\sqrt{N}} \int_a^b w(x)dx$$

- Where:

$$\text{var}_w g = \langle g^2 \rangle_w - \langle g \rangle_w^2$$

- Still goes like $N^{-1/2}$

Importance sampling for pathological function

- Let's return to the integral: $I = \int_0^1 \frac{x^{-1/2}}{e^x + 1} dx$
- Choose: $w(x) = x^{-1/2}$
- Then: $f(x)/w(x) = (e^x + 1)^{-1}$
  - Finite and well-behaved over the range
- Probability distribution is:

$$p(x) = \frac{x^{-1/2}}{\int_0^1 x^{-1/2} dx} = \frac{1}{2\sqrt{x}}$$

- So, using the transformation method:

$$\int_0^x \frac{1}{2\sqrt{x'}} dx' = \sqrt{x} = z \quad \Longrightarrow \quad x = z^2$$

Importance sampling for pathological function

- So finally, we need to sample:

$$I \simeq \frac{1}{N}\sum_{i=1}^{N}\frac{f(x_i)}{w(x_i)}\int_a^b w(x)dx = \frac{1}{N}\sum_{i=1}^{N}\frac{1}{e^{x_i}+1}\int_0^1 \frac{1}{\sqrt{x}}dx = \frac{1}{N}\sum_{i=1}^{N}\frac{2}{e^{x_i}+1}$$

- With the distribution $x = z^2$

Today's lecture:
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- Monte Carlo integration with divergences

- Monte Carlo simulation

Monte Carlo simulation

- Any computer simulation that uses random numbers to simulate physical process
- We saw a few examples already: radioactive decay and Rutherford scattering
- Used in every branch of physics
  - Particularly important in statistical mechanics and many-body physics

Monte Carlo simulation in stat mech

- Fundamental problem in statistical mechanics: Calculate expectation value of quantity of interest in thermal equilibrium

- Don't know the exact state of the system, only probability of occupying state *i* with energy E_i

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

- Then average value of observable *X*:

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

States with large numbers

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

- Calculating this sum exactly can only be done in a few specific systems (e.g., harmonic oscillator)
- Numerically challenging: states are order Avogadro's number in size
- E.g., one mole of gas with two states: total number of states is $2^{10^{23}}$
- Instead, use Monte Carlo approach to evaluate the sum

Monte Carlo approach to expectation values

- We could choose *N* terms in the sum at random to add up:

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

Needed to normalize the weighted average if not summing over *all* states

- This would not work well! Boltzmann probability is exponentially small for states $E_i \gg k_B T$

- Usually, most of the states are high energy, only a few contribute significantly

- **Need to use importance sampling!**

Importance sampling for thermal average

- Choose nonuniform distribution to focus on this small set
- Define weighted average over states:

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

- We choose: $g_i = X_i P(E_i)/w_i$
- So:

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

- Or:

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

Importance sampling for thermal average

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

- Evaluate by selecting *N* states randomly with nonuniform distribution:

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

Summed over all states

Summed over *N* samples

- Still need to choose w_i to bias us towards high-probability samples
  - Also, so that sum over all states *i* can be evaluated analytically

Weights for importance sampling

- Simple choice: $w_i = P(E_i)$
- Sums to 1 over all by definition
- Then we have:

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

- Thus, choose *N* states in proportion to their Boltzmann weights, and average *X* over them

Markov chain Monte Carlo

- Recall that: $$P(E_i) = \frac{e^{-\beta E_i}}{Z}, \qquad Z = \sum_i e^{-\beta E_i}$$

- Partition function requires a sum over all states that we are trying to avoid

- Can use a Markov chain to choose states with probability $P(E_i)$ without knowing the partition function:
  - Start with a state *i*
  - Generate a new state *j* by making a small change to *i*
  - Choice of new state is determined probabilistically by a set of transition probabilities T_{ij} that give probability for changing from state *i* to *j*

- If we chose T_{ij} correctly, probability of visiting any state on a step of the Markov chain is $P(E_i)$!

Transition probabilities in the MC

- We must end up in some state on every MC step, so:

$$\sum_j T_{ij} = 1$$

- Choose transition probabilities such that:

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

- I.e., choosing particular ratio of the probability to go from *i* to *j*, and *j* to *i*

- Partition function cancels out!

Transition probabilities in the MC

- If we have correct probability of being in a given state at one step, we will have the correct probability for all later steps
- To see this:
  - Suppose we find a set of T_{ij}'s that satisfy the previous conditions
  - Suppose the probability to be in state i on one particular step is $P(E_i)$
  - Then, probability to be in state j on the next step is:

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

- Once we get a Boltzmann distribution over states, we will keep it
  - Boltzmann distribution is a fixed point of the Markov chain
- Can also prove that we will converge to Boltzmann distribution
  - See, e.g., Appendix D of Newman

Metropolis-Hastings accept/reject

- Still have not worked out what elements of T_{ij} are
  - Actually, many possible choices
- Most common choice: Metropolis-Hastings algorithm:
  - Choose the change between *i* and *j* from specified set of possible changes
    - Can be, e.g., chosen at random, uniformly
  - Accept or reject the new state with acceptance probability:

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

  - I.e., definitely accept if energy is lowered (or equal); may still accept if energy is increased

Transition probabilities under Metropolis-Hastings

- Total probability to move from *i* to given *j* (if $E_j < E_i$)

$$T_{ij} = \frac{1}{M} e^{-\beta(E_j - E_i)}$$

Probability we accept

Probability we choose *j*

Transition probabilities under Metropolis-Hastings

- If $E_j > E_i$:

$$T_{ij} = \frac{1}{M} e^{-\beta(E_j - E_i)}, \quad T_{ji} = \frac{1}{M} \quad \Longrightarrow \quad \frac{T_{ij}}{T_{ji}} = e^{-\beta(E_j - E_i)}$$

- If $E_j \leq E_i$:

$$T_{ij} = \frac{1}{M}, \quad T_{ji} = \frac{1}{M} e^{-\beta(E_i - E_j)} \quad \Longrightarrow \quad \frac{T_{ij}}{T_{ji}} = e^{-\beta(E_j - E_i)}$$

- Thus, both consistent with :

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

Some comments about the Metropolis algorithm

- Note that many steps will not change the system
  - Still need to include in the sum
- The number of possible moves *M*, must be the same when going from *i* to *j* as *j* to *i*
- Moves must be chosen to get you to every state
  - Move set for which all states are accessible is called ergodic
- Will generally take some (unknown) time to equilibrate to Boltzmann distribution

Steps of Markov chain Monte Carlo:

- 1. Choose random starting state
- 2. Choose a move uniformly at random from set of moves
- 3. Calculate the acceptance probability
- 4. Accept or reject the move
- 5. Measure X in current state, add to sum
- 6. Go back to step 2

Example: Ideal gas

- Consider the quantum states of a particle or atom of mass *m* in cubic box of length *L*
- Energy of one particle given by:

Quantum numbers from 1 to infinity.

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

- Ideal gas: no interactions between particles
  - Energy is sum of individual particles:

$$E = \sum_{i=1}^{N} E(n_x^{(i)}, n_y^{(i)}, n_z^{(i)})$$

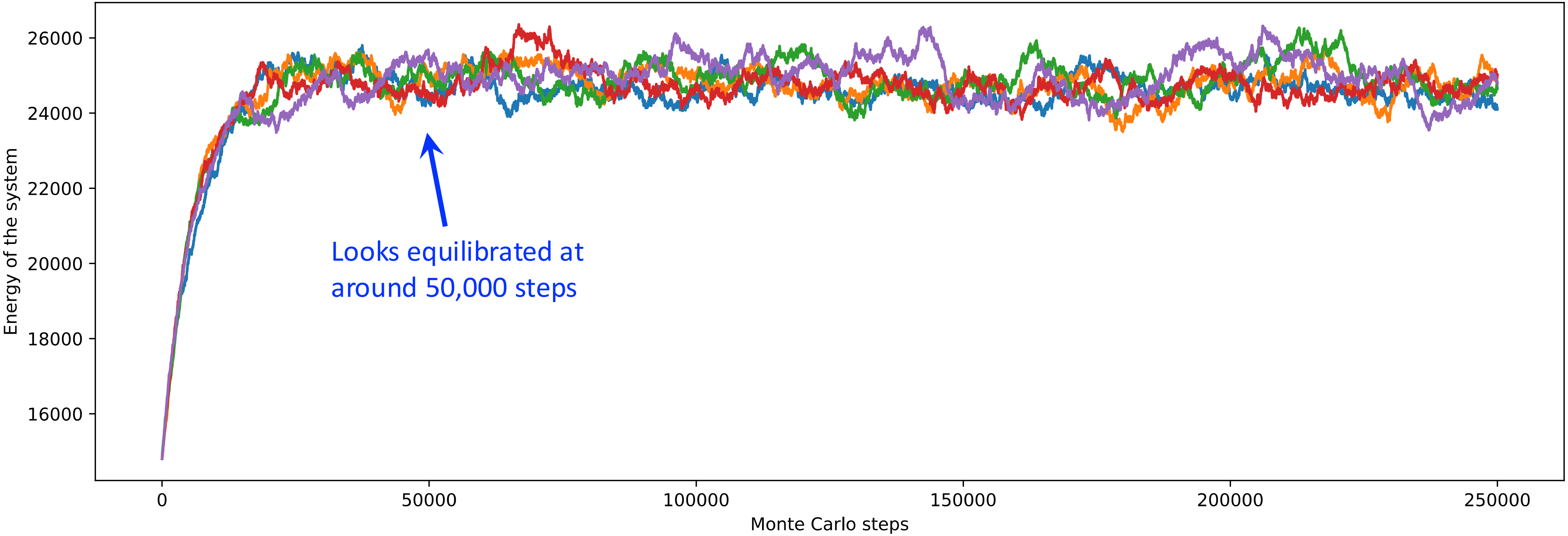
Move set for ideal gas

- Choose set of all moves of a single atom to one of the six "neighboring" states where n_x, n_y, or n_z differ by +/- 1
- Each Monte Carlo step, choose a random particle, chose a quantum number, change it by +/- 1
- Change in total energy just the change for single particle since there are no interactions
  - E.g., increase or decrease n_x of atom i by one:

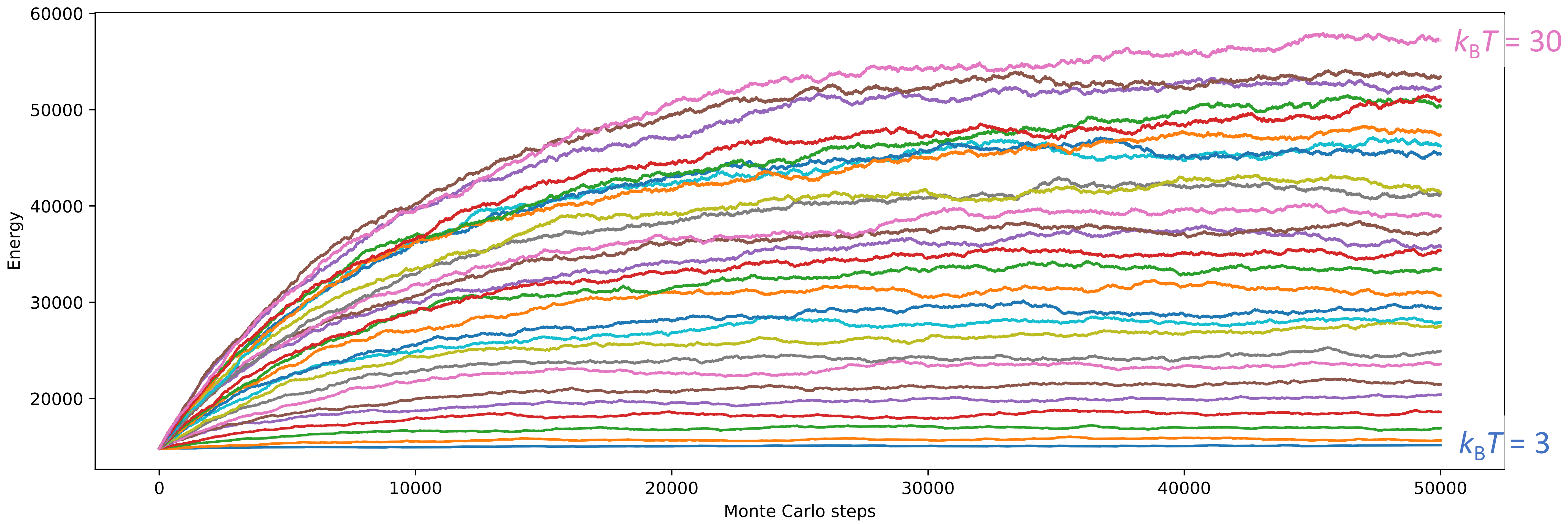
$$\begin{aligned}\Delta E &= \frac{\pi^2\hbar^2}{2mL^2}[(n_x \pm 1)^2 + n_y^2 + n_z^2] - \frac{\pi^2\hbar^2}{2mL^2}(n_x^2 + n_y^2 + n_z^2) \\ &= \frac{\pi^2\hbar^2}{2mL^2}[(n_x \pm 1)^2 - n_x^2] = \frac{\pi^2\hbar^2}{2mL^2}(\pm 2n_x + 1)\end{aligned}$$

- Note: Reject moves that try to make $n < 1$

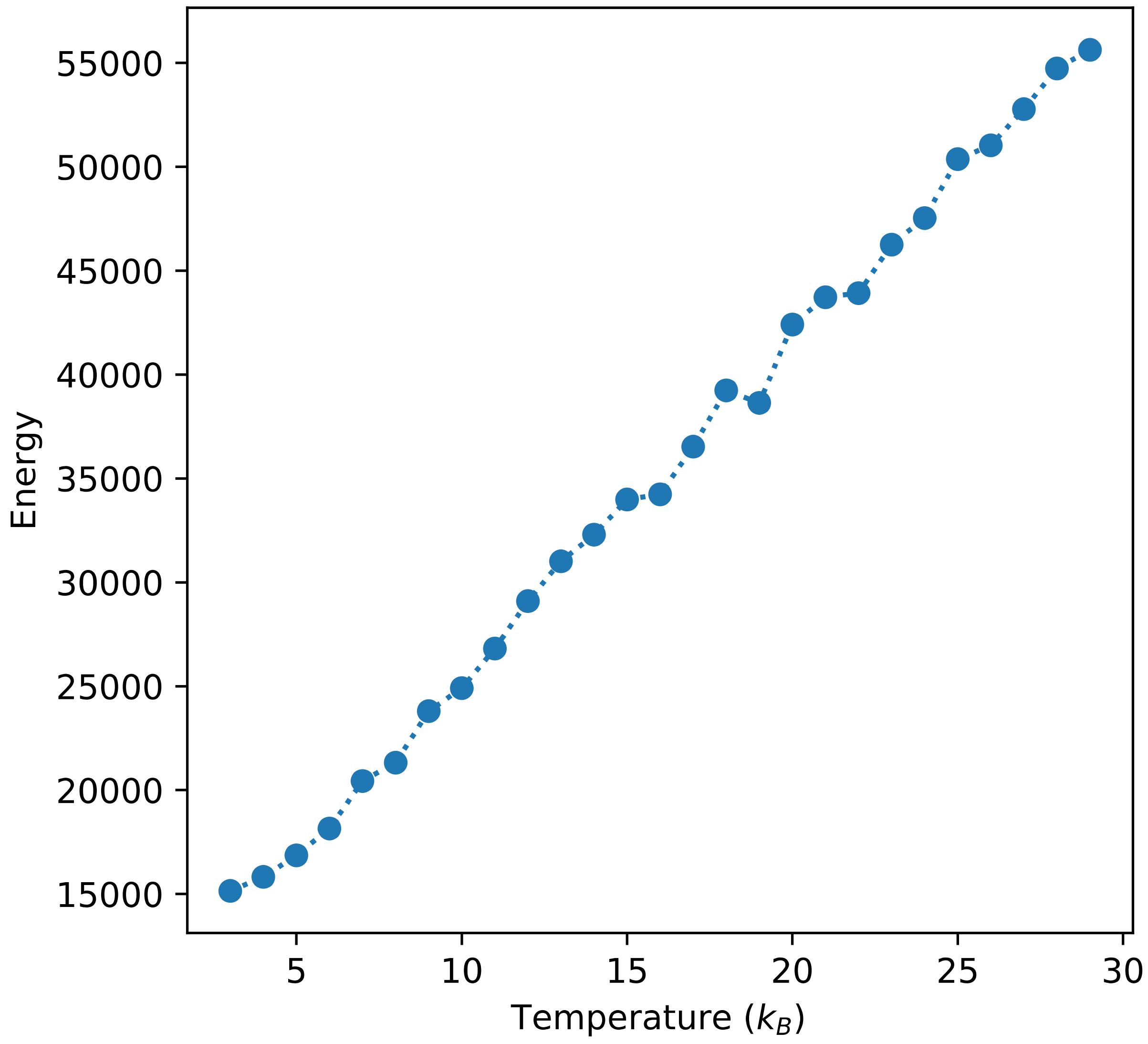
Monte Carlo simulation of ideal gas



Monte Carlo simulation of ideal gas: Dependence on T



Monte Carlo simulation of ideal gas: E vs. T



After class tasks

- Homework 5 is posted, due Nov. 19, 2025
- Almost done grading Homework 3

- Final project ideas due Nov. 19

- Readings:
  - Newman Sec. 10.3