Molecular Dynamics Simulations (and other work from Week 1)

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August 9, 2024

Outline

Problem 1: 1D Spring

- Potential energy: $U = \frac{k}{2}(x - x_0)^2$
- Force: $F = -k(x - x_0)$
- Implemented Verlet integration
- Observed energy conservation

Problem 1: Results

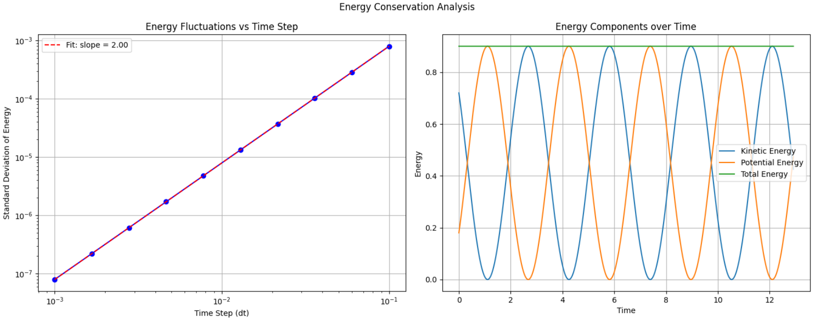

Figure: Energy components over time for 1D spring

Problem 2: Attracted Particles

- N soft disks with repulsive spring-like interaction
- Central attraction potential
- Total potential energy: $U = U_{int} + U_{center}$
- Implemented Verlet integration for 2D system

Problem 2: Animation of Particle Dynamics

Animation

of particle positions and total energy over time

Problem 2: Phase Space Visualization

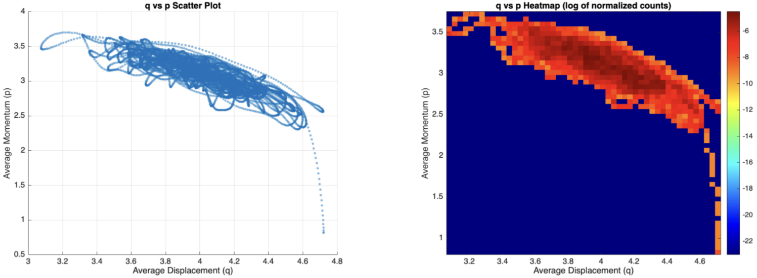

Figure: Left: q vs p scatter plot. Right: Phase Space Entropy heatmap

Proof: Energy Variance $O(dt^2)$

Theorem: The variance of the total energy in a Verlet integration scheme scales as $O(dt^2)$.
Proof:

- Let $E(t)$ be the true energy and $\tilde{E}(t)$ be the numerical approximation.
- The local truncation error of Verlet integration is $O(dt^4)$.
- Over $n = T/dt$ steps, the global error is $O(dt^3)$.
- Thus, $|\tilde{E}(t) - E(t)| = O(dt^3)$.

Proof: Energy Variance $O(dt^2)$ (cont.)

- The variance of $\tilde{E}(t)$ is given by:

$$\mathrm{Var}(\tilde{E}) = \mathbb{E}[(\tilde{E} - \mathbb{E}[\tilde{E}])^2]$$

- Since $E(t)$ is constant, $\mathrm{Var}(\tilde{E}) = \mathbb{E}[(\tilde{E} - E)^2]$
- From the previous slide, $(\tilde{E} - E)^2 = O(dt^6)$
- Therefore, $\mathrm{Var}(\tilde{E}) = O(dt^6)/dt^4 = O(dt^2)$

Markov Analysis: Introduction

- Perform a Markovian analysis on the energy time series
- Goal: Assess how well the energy dynamics can be described as a Markov process
- The discretized estimation error of a continuous system predicated on a many-body state space may exhibit Markovian properties

Mathematical Representation

- Let $\{H_t\}$ be the discrete-time stochastic process representing system energy
- Discretize energy values into n bins: $\{X_t\}$, where $X_t \in \{1, 2, ..., n\}$
- Markov property:

$$P(X_t = x_t | X_{t-1} = x_{t-1}, ..., X_0 = x_0) = P(X_t = x_t | X_{t-1} = x_{t-1})$$

Analysis Methodology

For each time gap k from 1 to maximum gap K:

1. Calculate one-step conditional probability matrix: $P_1(i,j) = P(X_t = j | X_{t-1} = i)$
2. Calculate k-step conditional probability matrix: $P_k(i,j) = P(X_t = j | X_{t-k} = i)$
3. Compute difference: $D_k = |P_k - P_1|$
4. Markovian score: $S_k = \frac{1}{n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} D_k(i,j)$

Plot S_k vs k to visualize Markovian behavior.

Estimation of Conditional Probabilities

We estimate conditional probabilities empirically:

$$\hat{P}_k(i,j) = \frac{N_k(i,j)}{\sum_j N_k(i,j)}$$

where $N_k(i,j)$ is the number of observed transitions from state i to state j with a time gap of k.

Interpretation of Results

- Perfect Markovian process: $S_k \approx 0$ for all k
- Somewhat Markovian process: S_k starts near 0 and gradually increases with k
- Rate of increase of S_k with k indicates deviation from Markovian behavior at longer time scales

Markov Analysis Results

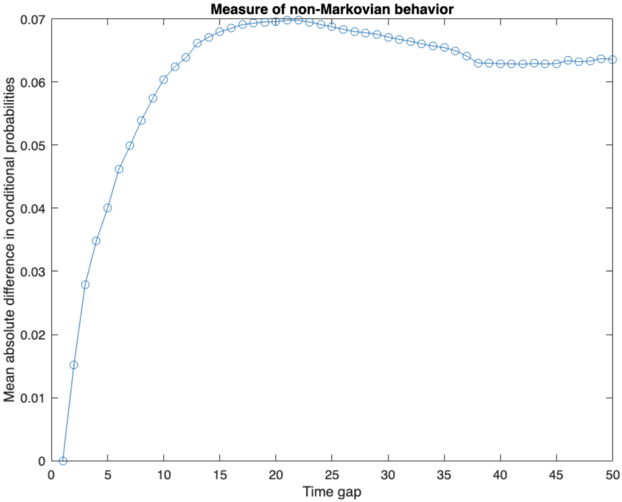

Figure: Markovian score S_k vs time gap k

Future Work: Empirical Temperature

- We have measurements for total E, P, V, and S at each time step
- Empirical temperature can be derived from the kinetic energy:

$$T = \frac{2K}{3Nk_B}$$

  where K is the total kinetic energy, N is the number of particles, and k_B is Boltzmann's constant
- Future analysis:
  - Temperature fluctuations over time
  - Relationship between T and other thermodynamic variables
  - Equilibration and ergodicity of the system

Conclusion

- Successfully implemented and analyzed 1D spring and 2D attracted particles systems
- Verified energy conservation and $O(dt^2)$ scaling of energy variance
- Future work will focus on empirical temperature analysis

Exploratory Reading: Geometric Error Metrics

- Ongoing exploration into geometric error metrics for numerical methods
- Based on an extension of the Shadowing Lemma (which I don't yet fully understand)
- Key concepts:
  - Symplectic manifolds representing true and approximate state spaces
  - True and approximate evolution operators
  - Optimal transformation between spaces
- Potential applications:
  - New approach to analyzing numerical errors in dynamical systems
  - Possible improvements in design of numerical methods
- Current status: Just for enrichment!