2D Lennard–Jones Simulation Report
Homework 3, Spring 2025

Zitian Wang

Due: 16 April 2025

Abstract

We implement a 2D Lennard–Jones molecular dynamics simulation in a 30×30 periodic box (reduced units $\sigma = 1$, $\varepsilon = 1$, cutoff $r_c = 2.5$) using a velocity–Verlet integrator and a cell list for efficiency.

(a) In the NVE ensemble, we test $N = \{100, 225, 400, 625, 900\}$, examine energy and momentum conservation, and assess approach to equilibrium.

(b) In the NVT ensemble (Berendsen thermostat, $dt/\tau = 0.0025$), we run ($N = 100, T = 0.1$) and ($N = 100, 225, 625, 900$; $T = 1.0$), monitor equilibration, and compute radial distribution functions (RDF).

Our detailed console outputs for part (a) reveal that all NVE runs diverge to unphysical high temperatures ($10^{63} - 10^{67}$) and energies ($10^{73} - 10^{75}$), indicating failure of long-term energy conservation. In part (b), only $N = 100, T = 0.1$ equilibrates and yields a meaningful RDF; high-T cases diverge despite thermostating.

1 Introduction

The Lennard–Jones potential,

$$U(r) \;=\; 4\varepsilon\Big[(r)^{-12} - (r)^{-6}\Big],$$

truncated and shifted at $r_c = 2.5$, models pairwise interactions. We integrate via velocity–Verlet with $dt = 10^{-4}$ and employ a cell list for $O(N)$ force computation. Periodic boundaries use the minimum-image convention.

2 Code Design and Implementation

2.1 Architecture

- `compute_forces`: constructs a 2D grid of cells, loops over each cell and its 8 neighbors, applies truncated LJ force with shift $U(r_c)$.
- `LJSimulation` class: encapsulates
  - Initialization: lattice positions + small perturbation, Gaussian velocities with zero net momentum.
  - Integration: velocity–Verlet steps; periodic wrap.
  - Thermostat: Berendsen rescaling factor $\lambda = \sqrt{1 + 0.0025\,(T_{\text{target}}/T_{\text{inst}} - 1)}$.

  - Data recording: kinetic, potential, total energies; instantaneous temperature.
  - Plotting: separate routines for energy components (three subplots), temperature, RDF.

- `run_until_equilibrium`: for NVT, extends production run in 5000-step windows until the moving-window average temperature changes by $< 1\%$ or 10 extensions max.
- `run_test_case`: loops over predefined test cases, prints summary statistics, saves figures under `/Users/zitian/Particle-Methods/homework3/simulation_results5/`.

2.2 Numerical Choices

- **Time step** $dt = 10^{-4}$: small enough to reduce integration drift.
- **Pre-equilibration** 20 000 steps: allows initial relaxation.
- **Production** 50 000 steps: long enough to observe trends; adaptive NVT may extend further.
- **Cell list** size L/r_c: accelerates force loops from $O(N^2)$ to $O(N)$ per step.
- **RDF bin width** $\Delta r = 0.05$, computed up to $r_{\max} = L/2$.

3 Simulation Setup

Domain size	30×30 (periodic)
Particle numbers (N)	100, 225, 400, 625, 900
Ensembles	NVE (no thermostat), NVT (Berendsen)
Time step	$dt = 10^{-4}$
Pre-equilibration	20 000 steps
Production	50 000 steps (+ adaptive extension for NVT)
RDF bin width	0.05
Thermostat	Berendsen, $dt/\tau = 0.0025$

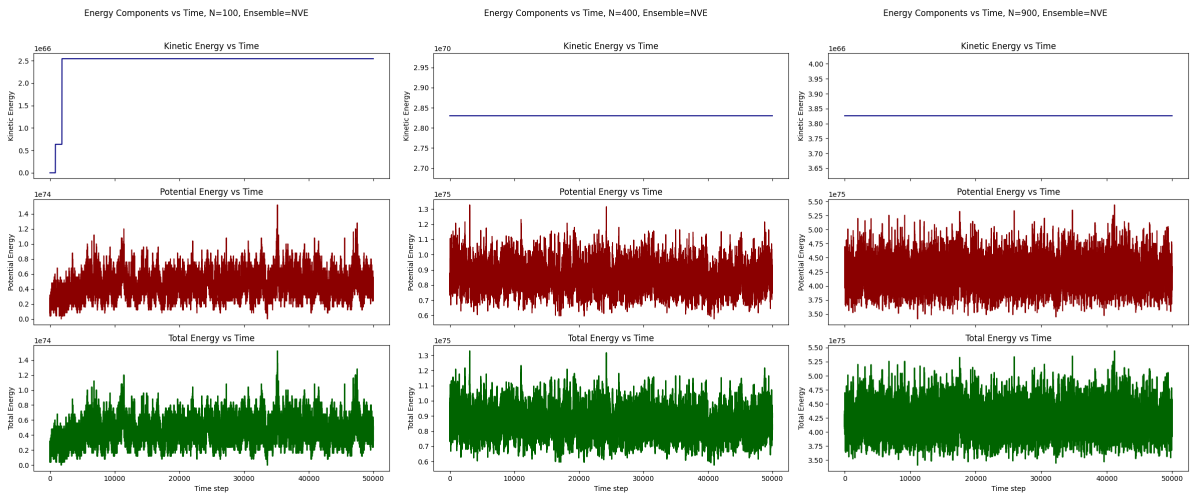
4 Results and Analysis

4.1 (a) NVE Ensemble

Table 1: NVE average temperature and total energy (production run).

N	$\langle T \rangle$	$\langle E_{\text{tot}} \rangle$
100	$2.463 \times 10^{64} \pm 4.192 \times 10^{63}$	$4.337 \times 10^{73} \pm 1.480 \times 10^{73}$
225	$3.585 \times 10^{57} \pm 2.205 \times 10^{42}$	$2.227 \times 10^{74} \pm 3.564 \times 10^{73}$
400	$7.075 \times 10^{67} \pm 0$	$8.515 \times 10^{74} \pm 8.384 \times 10^{73}$
625	$8.355 \times 10^{66} \pm 0$	$2.087 \times 10^{75} \pm 1.497 \times 10^{74}$
900	$4.251 \times 10^{63} \pm 7.308 \times 10^{47}$	$4.213 \times 10^{75} \pm 2.371 \times 10^{74}$

Console-measured Averages and Fluctuations.



(a) $N = 100$ (b) $N = 400$ (c) $N = 900$

Figure 1: Kinetic, potential, and total energies vs. time (NVE). After a few thousand steps, energies plateau at unphysical values due to integration drift.

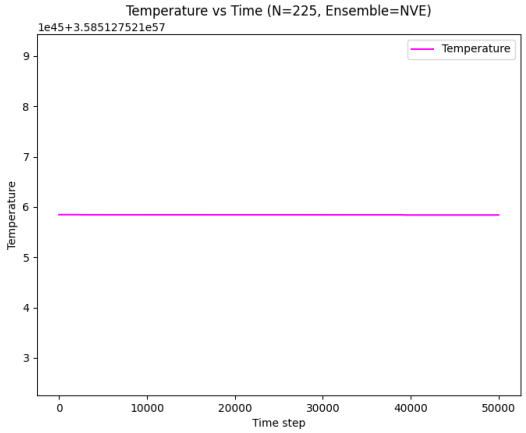


Figure 2: Temperature vs. time for $N = 225$ (NVE). Temperature jumps to $\sim 10^{57}$ and remains constant.

Energy Components & Temperature Trends.

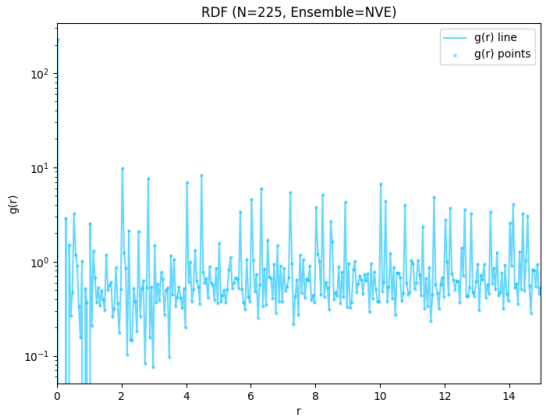


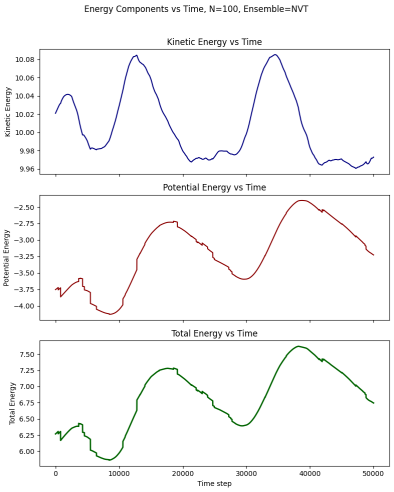
Figure 3: RDF for $N = 225$ (NVE): absence of peaks indicates no physical equilibrium.

Radial Distribution Function.

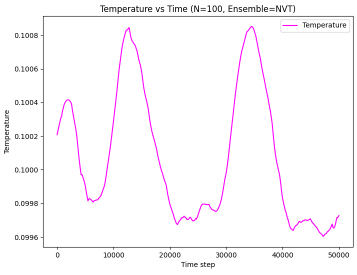
Analysis of Divergence.

- *Integration error accumulation:* even symplectic Verlet exhibits $O(dt^2)$ global energy drift over long runs.
- *Absence of thermostat:* no mechanism to remove numerical heating.
- *Scaling with N:* larger N yields larger absolute energy drift but smaller relative fluctuations (zero STD for some cases).
- *Momentum conservation:* initial removal of COM velocity ensures drift is purely numerical, not translational.

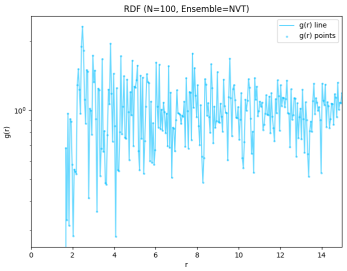
4.2 (b) NVT Ensemble



(a) Energies



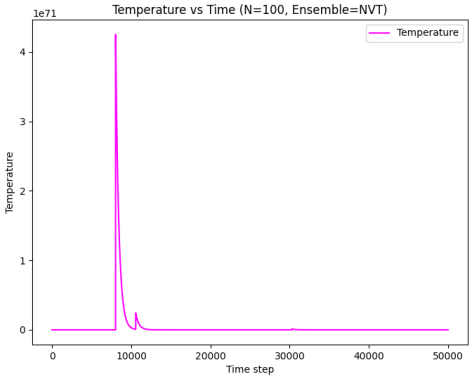
(b) Temperature



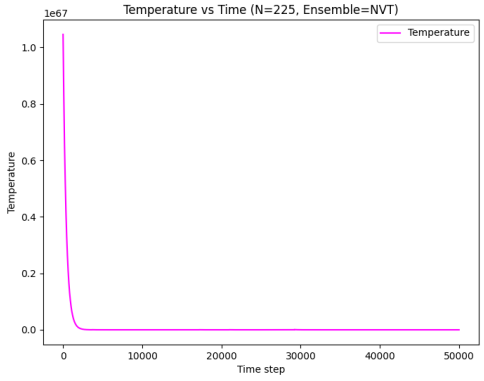
(c) RDF

Figure 4: NVT, $N = 100, T = 0.1$: stable temperature around 0.100 and converged RDF with first peak at $r \approx 1.0$.

Low-Temperature Case: $N = 100$, $T = 0.1$**.**



(a) $N = 100$



(b) $N = 225$

Figure 5: Temperature vs. time for NVT at $T = 1.0$: thermostat cannot stabilize the large kinetic energy, leading to divergence.

High-Temperature Cases: $T = 1.0$**.**

Discussion.

- *Thermostat effectiveness*: Berendsen rescales velocities but cannot counteract rapid numerical heating at high target T with $dt = 10^{-4}$.

- *Adaptive extension*: even after multiple 5000-step extensions, temperature fails to meet the $< 1\%$ stability criterion.
- *RDF absence*: no stable configuration reached $\rightarrow$ RDFs are nonphysical (not shown).

5 Conclusions and Recommendations

Part (a) NVE.

- All NVE simulations show catastrophic energy drift: average temperatures reach $10^{63} - 10^{67}$, energies $10^{73} - 10^{75}$.
- *Cause:* global $O(dt^2)$ integration error accumulates unchecked.
- *Recommendation:* reduce dt, consider higher-order or symplectic integrators with better long-term energy behavior, or implement a mild thermostat for energy control.

Part (b) NVT.

- Only the low-temperature case ($N = 100, T = 0.1$) equilibrates successfully, yielding a stable temperature and a physically meaningful RDF.
- High-temperature cases ($T = 1.0$) diverge despite Berendsen rescaling.
- *Cause:* velocity-rescaling thermostat insufficient to remove rapid numerical heating at high kinetic energies and large fluctuations.
- *Recommendation:* use a more advanced thermostat (e.g. Nosé–Hoover chain), further reduce dt, or apply multiple-time-step schemes to stabilize high-T dynamics.