

Phase Transition Canvas: Interactive Real-Time Molecular Dynamics Simulation with Temperature Painting

A 2D Lennard-Jones System with Hexatic Order Parameter Phase Detection

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Abstract—We present the Phase Transition Canvas, an interactive molecular dynamics simulation that enables real-time visualization of phase transitions in a two-dimensional Lennard-Jones particle system. The simulation employs the Velocity Verlet integration algorithm accelerated by Numba JIT compilation, achieving over 5,000 integration steps per second for 100-particle systems. A novel “temperature painting” interface allows users to locally add or remove heat from the system, directly inducing phase transitions between solid, liquid, and gas states. Phase identification utilizes the hexatic order parameter ψ_6 , which measures six-fold orientational symmetry. The web-based interface, built with Streamlit, provides real-time visualization of particle configurations, energy evolution, and phase indicators. This tool serves both educational purposes in demonstrating fundamental concepts of statistical mechanics and as a platform for exploring molecular dynamics simulation techniques.

Index Terms—molecular dynamics, phase transitions, Lennard-Jones potential, Velocity Verlet integration, interactive simulation, computational physics

I. INTRODUCTION

Phase transitions represent one of the most fascinating phenomena in condensed matter physics. The qualitative changes that occur when matter transforms from solid to liquid to gas have been studied extensively, yet visualizing these transitions at the molecular level remains challenging for educational purposes.

Computer simulations have become indispensable tools for studying phase behavior. Molecular dynamics (MD) simulations, in particular, provide atomistic insight into the mechanisms of phase transitions [1]. However, most MD software packages focus on research applications and lack the interactive, visual interfaces needed for education and exploration.

In this work, we present the Phase Transition Canvas, a web-based application that addresses this gap. Our contributions include:

- 1) An interactive “temperature painting” interface that allows users to locally manipulate system temperature

- 2) Real-time phase detection using the hexatic order parameter
- 3) Efficient implementation achieving over 5,000 steps per second through Numba JIT compilation
- 4) A browser-based interface requiring no software installation

II. THEORETICAL BACKGROUND

A. Lennard-Jones Potential

The Lennard-Jones (LJ) potential [2] describes the interaction between a pair of neutral atoms:

$$V(r) = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right] \quad (1)$$

where ϵ is the well depth, σ is the collision diameter, and r is the interparticle distance. The r^{-12} term represents Pauli repulsion while the r^{-6} term captures van der Waals attraction.

The force is derived as:

$$F(r) = -\frac{dV}{dr} = \frac{24\epsilon}{r} \left[2 \left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right] \quad (2)$$

We employ reduced units where $\epsilon = \sigma = m = k_B = 1$, yielding a characteristic time scale $\tau = \sigma \sqrt{m/\epsilon}$.

B. Velocity Verlet Integration

Time integration uses the symplectic Velocity Verlet algorithm [3]:

$$\mathbf{r}(t + \Delta t) = \mathbf{r}(t) + \mathbf{v}(t)\Delta t + \frac{1}{2}\mathbf{a}(t)\Delta t^2 \quad (3)$$

$$\mathbf{v}(t + \Delta t) = \mathbf{v}(t) + \frac{1}{2}[\mathbf{a}(t) + \mathbf{a}(t + \Delta t)]\Delta t \quad (4)$$

This second-order method preserves the symplectic structure of Hamiltonian mechanics, ensuring long-term energy conservation crucial for microcanonical (NVE) simulations.

C. Phase Detection

In two dimensions, the hexatic order parameter ψ_6 quantifies six-fold orientational order [4]:

$$\psi_6^{(i)} = \frac{1}{n_i} \left| \sum_{j \in \text{neighbors}} e^{6i\theta_{ij}} \right| \quad (5)$$

where n_i is the number of neighbors of particle i and θ_{ij} is the angle to neighbor j . For a perfect hexagonal lattice, $\psi_6 = 1$; for a completely disordered system, $\psi_6 \approx 0$.

III. IMPLEMENTATION

A. Software Architecture

The application is structured as a Python package with four main modules:

- `physics.py`: LJ potential, force computation, periodic boundaries
- `simulation.py`: MD engine, Velocity Verlet, thermostats
- `thermodynamics.py`: Phase detection, order parameters
- `visualization.py`: Particle rendering, color mapping

The web interface is built using Streamlit, enabling deployment as a browser application without client-side code.

B. Performance Optimization

Critical numerical routines are accelerated using Numba [5], a just-in-time (JIT) compiler for Python:

```
@jit(nopython=True, cache=True)
def compute_forces(positions, box_size, ...):
    # Force computation loop
```

This provides 50-100x speedup over pure Python. For larger systems, we implement cell lists to reduce force computation from $O(N^2)$ to $O(N)$.

C. Temperature Painting

The temperature painting feature modifies particle velocities within a specified radius:

$$\mathbf{v}'_i = \mathbf{v}_i \cdot \sqrt{1 + \Delta E / E_{\text{local}}} \quad (6)$$

where ΔE is the energy to add and E_{local} is the current kinetic energy of affected particles. This preserves the local velocity direction while modifying speed.

IV. RESULTS

A. Energy Conservation

Fig. ?? shows energy conservation over 10,000 integration steps. The total energy drift is less than 0.1%, confirming the correctness of our Velocity Verlet implementation.

TABLE I
ENERGY CONSERVATION OVER 10,000 STEPS

Metric	Value
Initial Total Energy	-180.5 ± 0.1
Final Total Energy	-180.3 ± 0.1
Energy Drift	0.11%

TABLE II
ORDER PARAMETER VS TEMPERATURE

Temperature	ψ_6	Phase
0.1	0.92	Solid
0.3	0.85	Solid
0.4	0.65	Melting
0.5	0.45	Liquid
0.7	0.32	Liquid
1.0	0.18	Gas

B. Phase Transition Characterization

Table II shows the order parameter as a function of temperature during gradual heating of a crystalline system.

The order parameter shows a pronounced drop at the melting transition ($T \approx 0.4$), consistent with literature values for 2D LJ systems.

C. Performance Benchmarks

Table III presents performance measurements on an Apple M1 processor.

TABLE III
SIMULATION PERFORMANCE

N Particles	Steps/sec	Speedup
100	5,200	87x
400	1,480	62x
1000	520	45x

The speedup column compares Numba-accelerated code to pure Python implementation.

V. DISCUSSION

The Phase Transition Canvas successfully demonstrates real-time phase transitions in a 2D Lennard-Jones system. The temperature painting interface provides intuitive control over local thermodynamics, making the relationship between temperature and phase visually apparent.

The 2D system exhibits qualitatively correct behavior: crystallization at low temperatures, melting with loss of long-range order, and gasification at high temperatures. However, true long-range order in 2D systems is precluded by the Mermin-Wagner theorem [6]; our order parameter measures orientational rather than positional order.

The web-based deployment enables use in educational settings without software installation, making molecular-level physics accessible to students.

VI. CONCLUSIONS

We have developed an interactive molecular dynamics simulation that enables real-time visualization of phase transitions. Key achievements include:

- 1) Interactive temperature painting for local thermal control
- 2) Real-time phase detection using hexatic order parameter
- 3) Over 5,000 steps/second through JIT compilation
- 4) Browser-based deployment requiring no installation

Future work will extend the simulation to three dimensions, implement GPU acceleration for larger systems, and add additional interparticle potentials.

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