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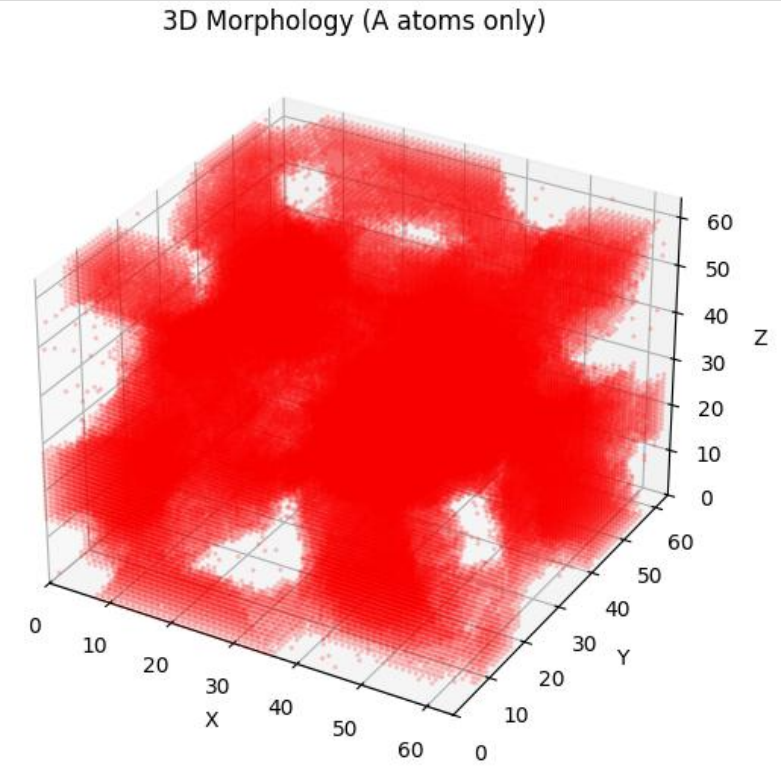

Computational Physics – Project 15.45

Vacancy mediated dynamics in binary alloys

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Content

Introduction

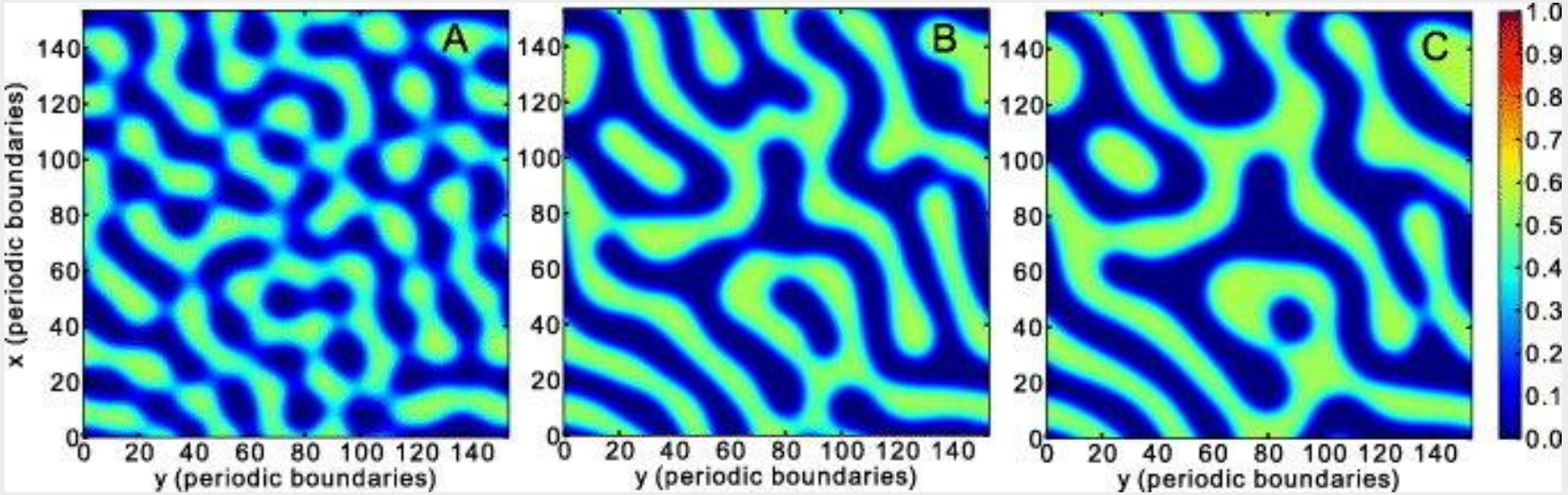
1. Spinodal Decomposition

When a binary alloy is rapidly quenched from a high temperature to a low temperature unstable state ($< T_c$), a pattern of domain formation called spinodal decomposition takes place as the two metals in the alloy separate.

2. Lifshitz-Slyozov Law

In the late stage of phase separation, the linear dimension R of domains exhibits power-law scaling with time t, a phenomenon universally applicable in two-dimensional and higher-dimensional systems.

$$R(t) \sim t^{1/3}$$



Problem Description

(a) initial state (random placement)

(b) Domain Size $R-t$ relations ($t=2^n$)

- pair correlation function $C(r)=<s_i s_j>$
- energy formula $R=\frac{2}{2+<E>/N}$

(c) temperature effects

(d) dimension effects

Model & Theory

- Ising Model

$$H = -J \sum_{\langle i,j \rangle} S_i S_j$$

$\langle i,j \rangle$： Sum over all nearest-neighbor grid points

$S_i \in \{+1(\mathrm{A}), -1(\mathrm{B}), 0(\mathrm{Vacancy})\}$

$J > 0$： Ferromagnetic interaction constant

- Metropolis Algorithm

$$P(\text{accept}) = \min\left(1, e^{-\frac{\Delta E}{k_B T}}\right)$$

$$\Delta E = E_{\text{new}} - E_{\text{old}}$$

Model & Theory

- Measure of Domain Size $R(t)$:

A. Pair Correlation Function

$$C(r) = \langle S_i \, S_{i+r} \rangle$$
$$C(R_{corr}) = 0$$

B. Energy-based Method

$$R_E = \frac{2}{(\langle E \rangle / N)/J + 2}$$

Implementation - Initialize Lattice

```
20  // initialize_lattice
21  void initialize_lattice(vector<int>& lattice, int L, int& vacancy_pos, mt19937& g) {
22      int N = L * L;
23      vector<int> atoms;
24      for (int i = 0; i < N / 2; ++i) { atoms.push_back(1); atoms.push_back(-1); }
25      shuffle(atoms.begin(), atoms.end(), g);
26      lattice = atoms;
27      uniform_int_distribution<int> dist(0, N - 1);
28      vacancy_pos = dist(g);
29      lattice[vacancy_pos] = 0; // insert vacancy
30  }
```

Generate equal quantities of A and B atoms

Random placement

Insert vacancy

Implementation - Metropolis Algorithm

```cpp
// local energy calculation
double get_local_energy(const vector<int>& lattice, int idx, int L, double J) {
    if (lattice[idx] == 0) return 0.0;
    int x = idx / L, y = idx % L;
    int neighbors[] = {get_idx(x+1, y, L), get_idx(x-1, y, L), get_idx(x, y+1, L),
    get_idx(x, y-1, L)};
    double energy = 0;
    for (int n : neighbors) {
        if (lattice[n] != 0) energy += (lattice[idx] == lattice[n]) ? -J : J;
    }
    return energy;
}
```

To improve efficiency, we calculate only the **local energy difference** involving exchange, rather than the total system energy.

Vacancy do not contribute to the interaction energy.

```cpp
    for (int mcs = 0; mcs <= num_mc; ++mcs) {
        // Monte Carlo Steps
        for (int step = 0; step < L * L; ++step) {
            int dir = uniform_int_distribution<int>(0, 3)(gen);
            int vx = vacancy_pos / L, vy = vacancy_pos % L;
            int nx = vx, ny = vy;
            if (dir == 0) nx++; else if (dir == 1) nx--; else if (dir == 2) ny++; else ny--;
            int neighbor_idx = get_idx(nx, ny, L);

            double e_old = get_local_energy(lattice, neighbor_idx, L, J);
            swap(lattice[vacancy_pos], lattice[neighbor_idx]);
            double e_new = get_local_energy(lattice, vacancy_pos, L, J);
            double dE = e_new - e_old;

            if (dE <= 0 || uniform_real_distribution<double>(0, 1)(gen) < exp(-dE / T)) {
                current_energy += dE;
                vacancy_pos = neighbor_idx;
            } else {
                swap(lattice[vacancy_pos], lattice[neighbor_idx]);
            }
        }
```

In each *MCS*, $L \times L$ attempts are made.
Each attempt switches the *vacancy* with one random neighbor, and the acceptance of this move is determined by the *Metropolis Algorithm*.

Implementation – 3D Circumstance

Adjustments:

1. **Coordinates**

$$(x, y) \rightarrow (x, y, z)$$

Coordination Number

$$z = 4 \rightarrow z = 6$$

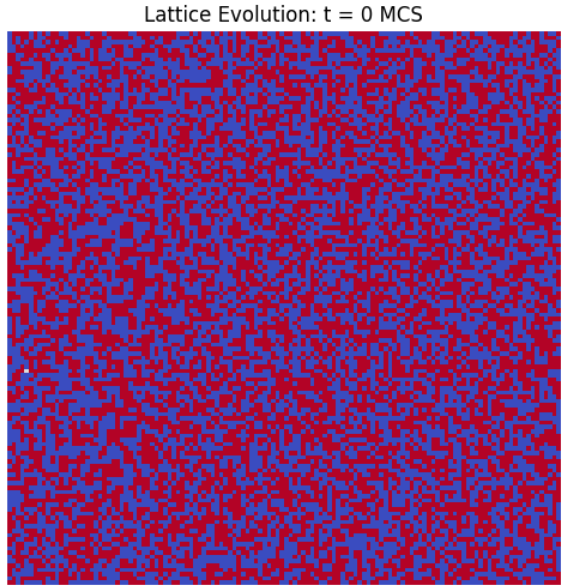
Neighbors: Up, Down, Left, Right, Front, Back

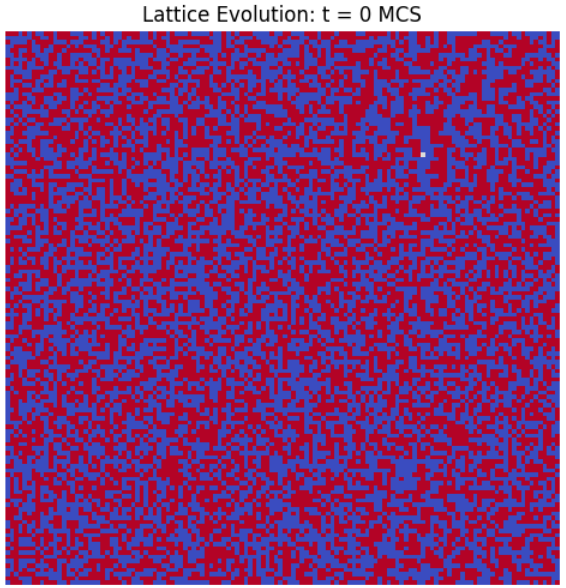
2. **Formula**

$$R_{E_{2D}} = \frac{2}{(\langle E \rangle / N)/J + 2} \rightarrow R_{E_{3D}} = \frac{3}{(\langle E \rangle / N)/J + 3}$$

Microstructure Evolution

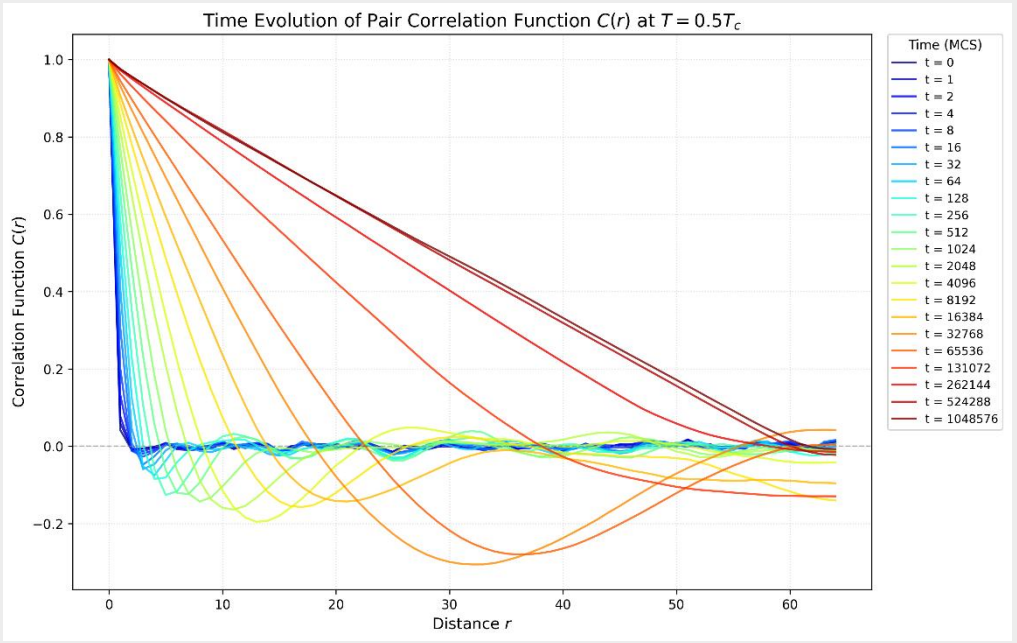
$$T = 0.5T_c$$

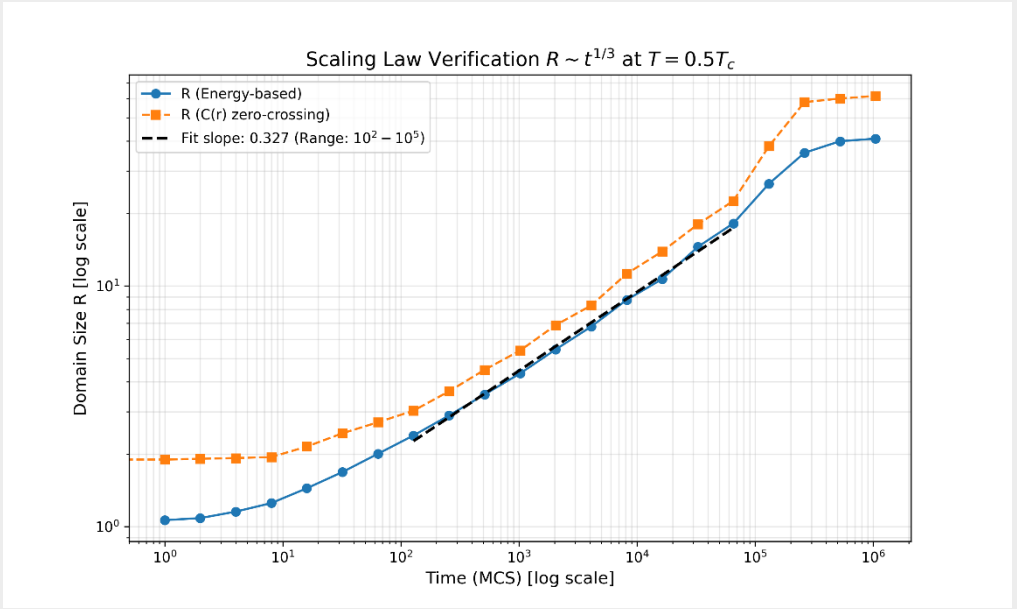




Spinodal Decomposition → Coarsening → Saturation

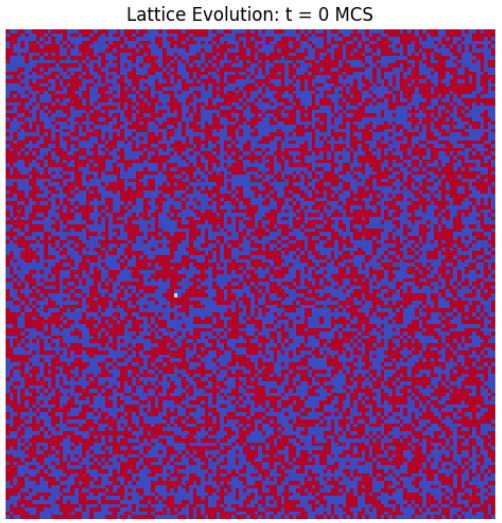
Total: $2^{20} = 1048576MCS$

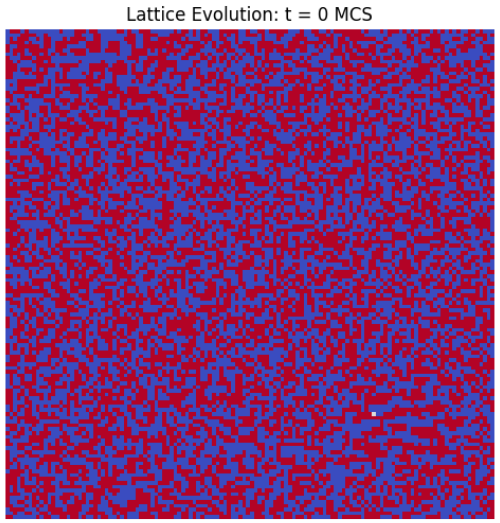


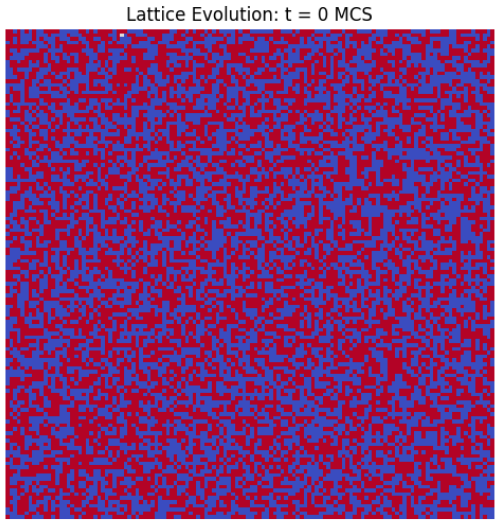


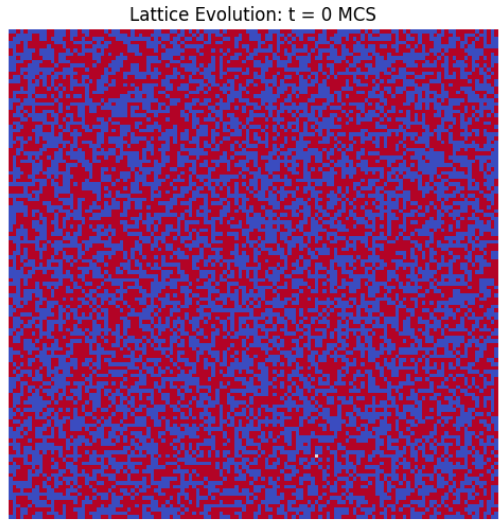
$n \approx 0.327$

Temperature Effects









$T = 0.2T_c$ $T = 0.7T_c$

Phase separation

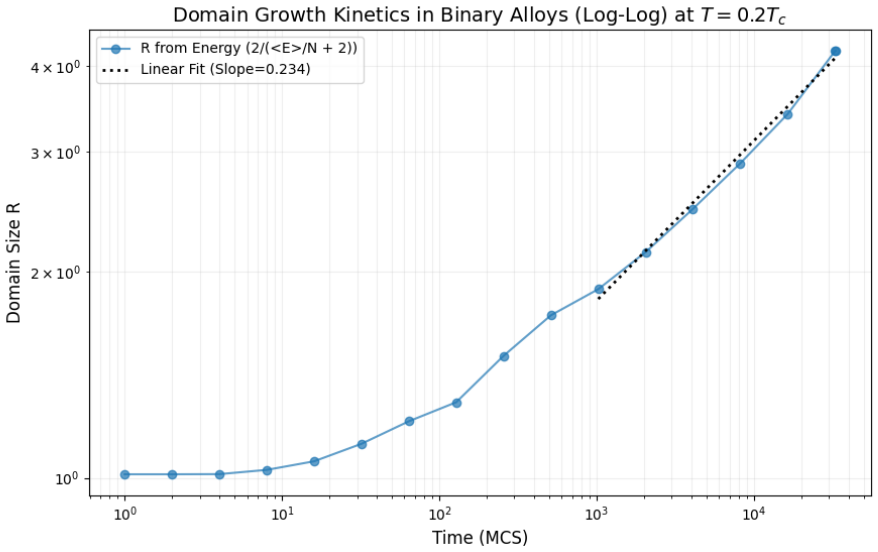
$T = 1.0T_c$

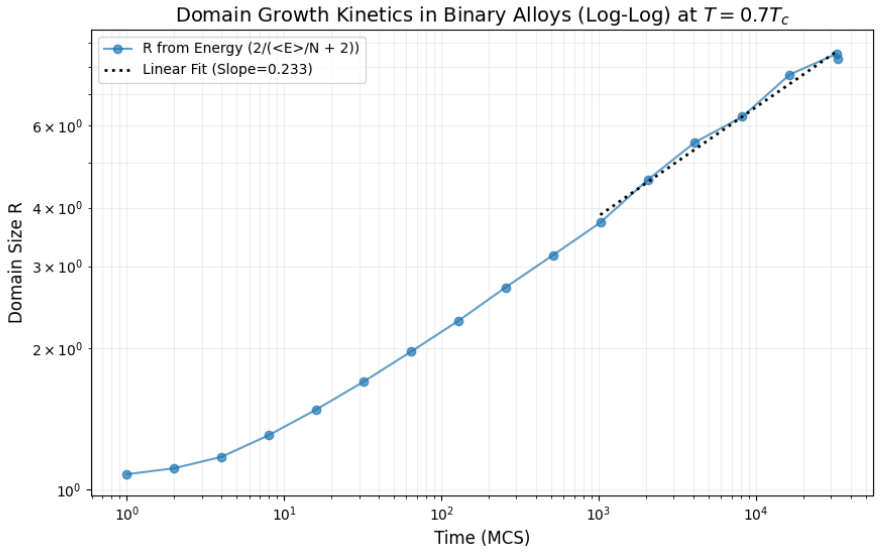
Critical

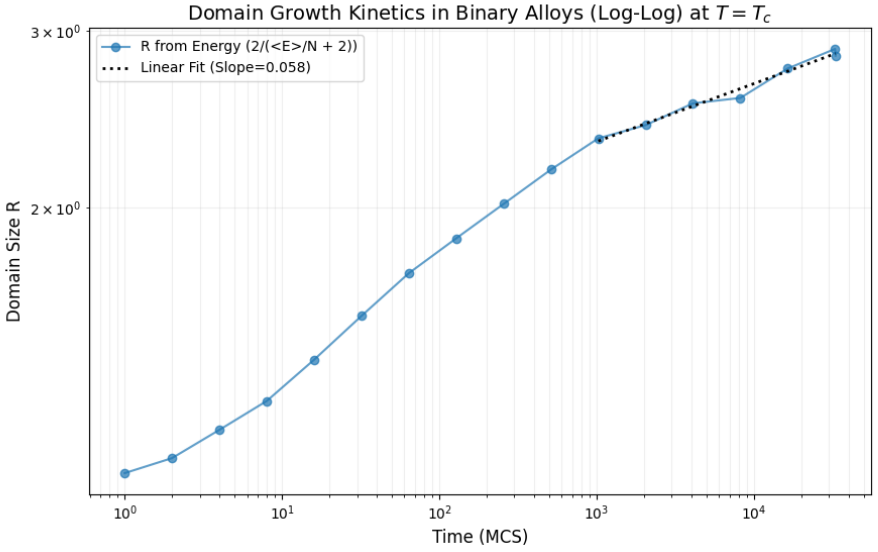
$T = 1.5T_c$

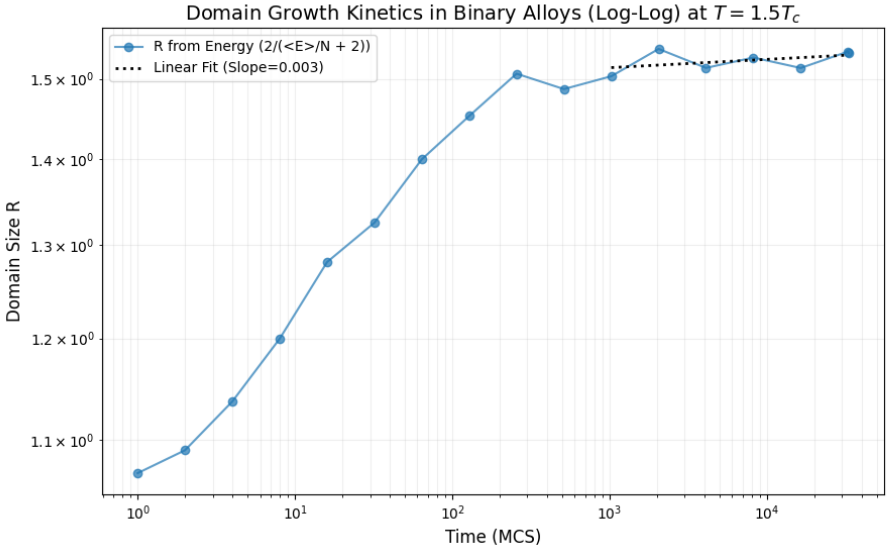
Disordered

Temperature Effects – Domain Growth

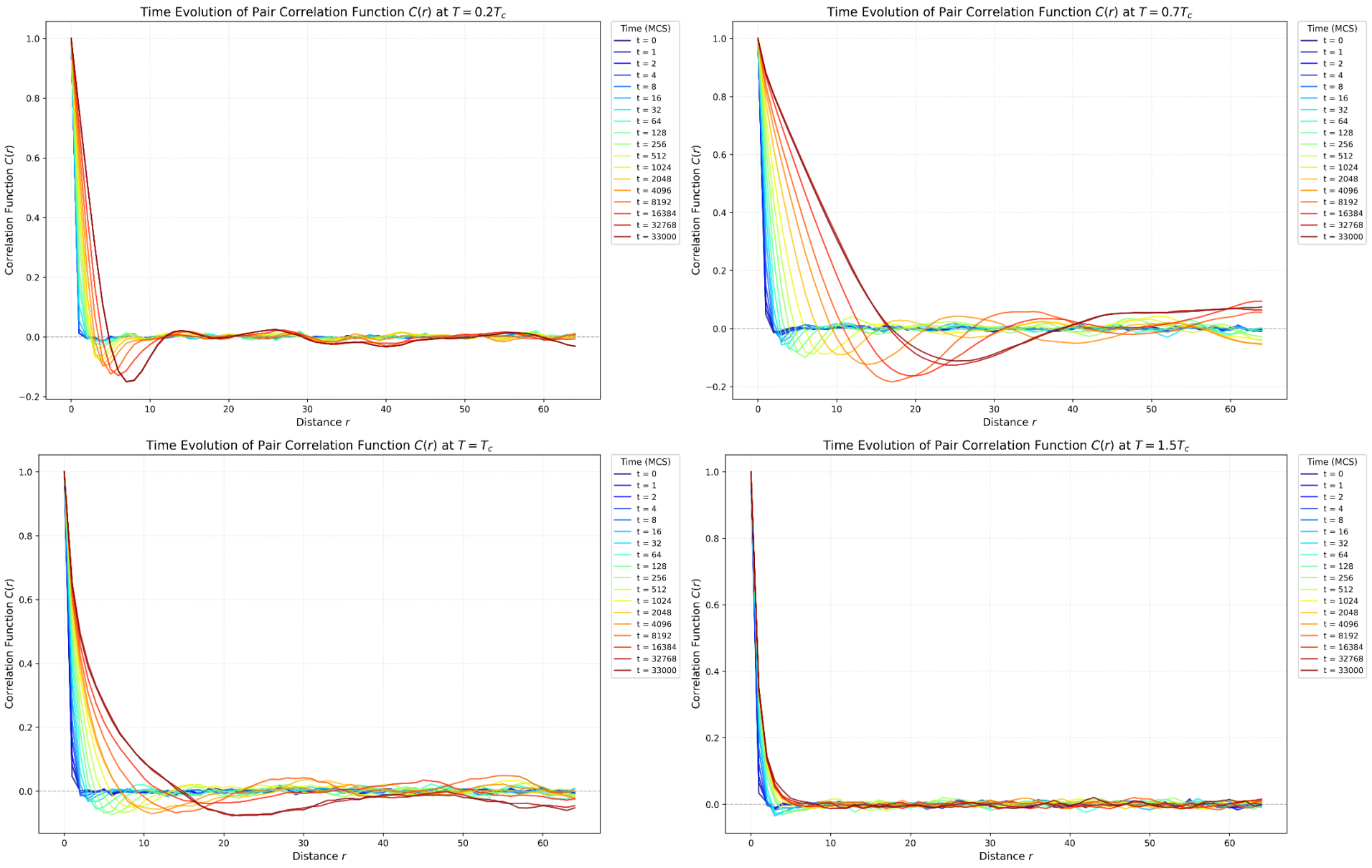




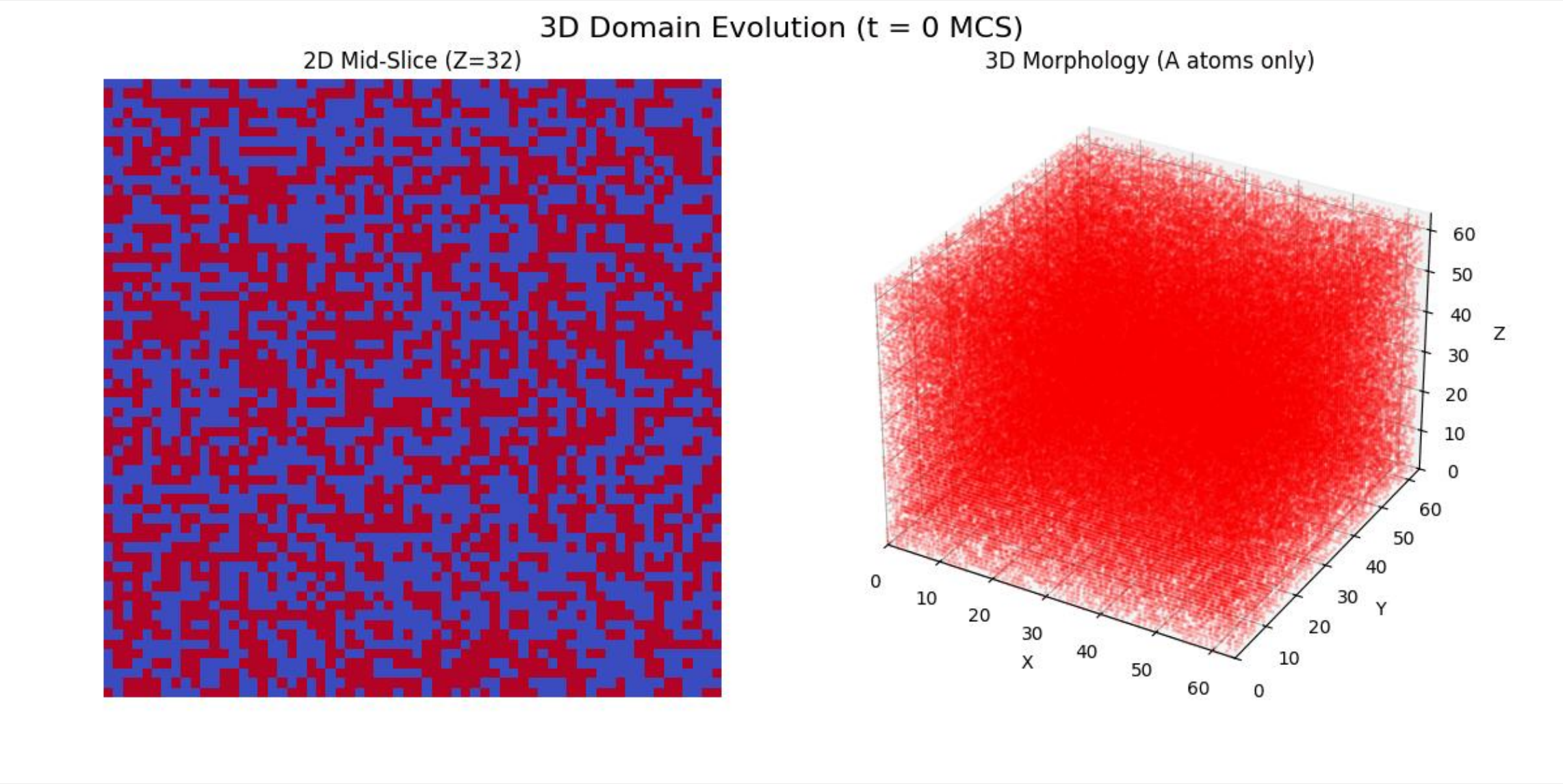




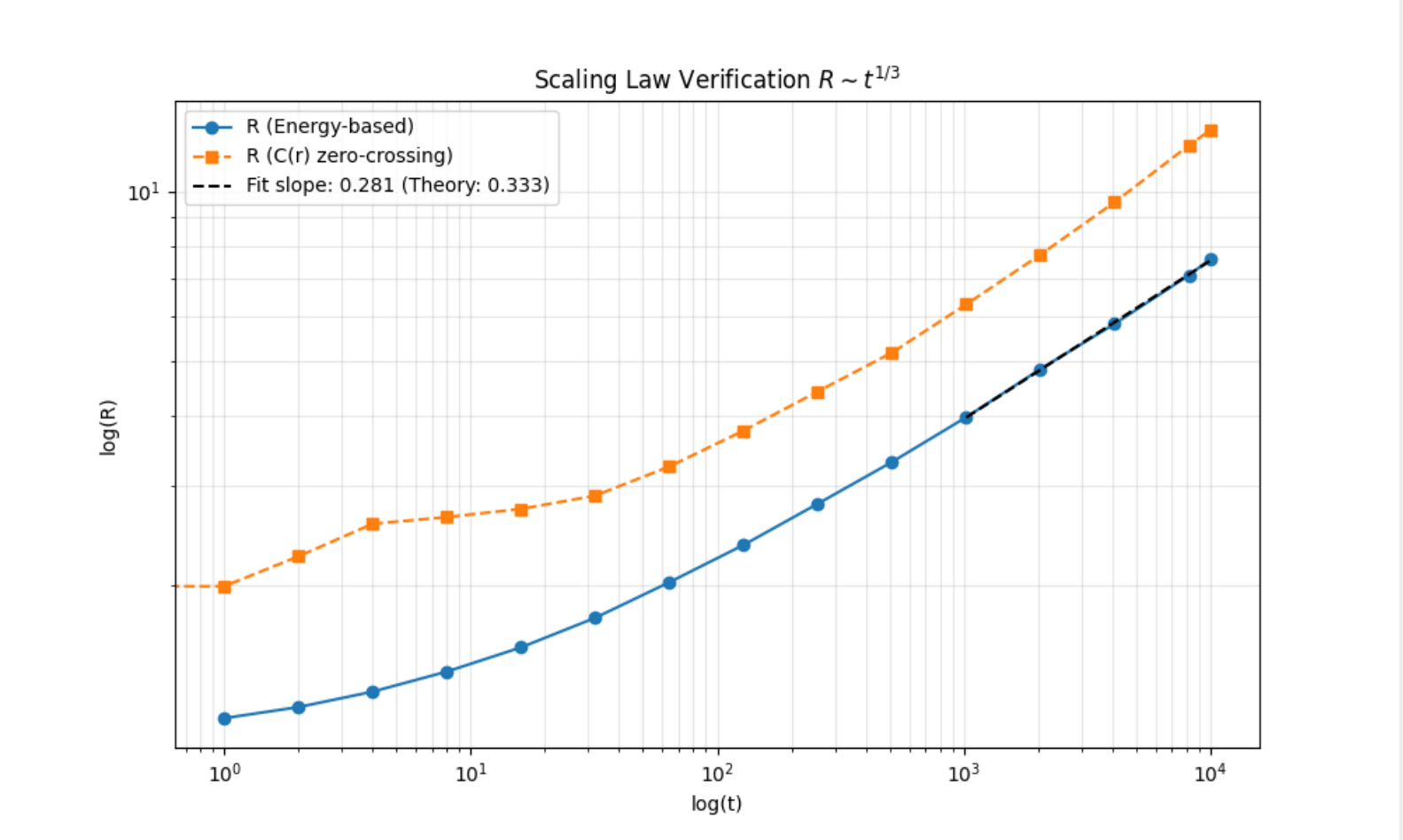
Temperature Effects – Pair Correlation Function



3D Simulation



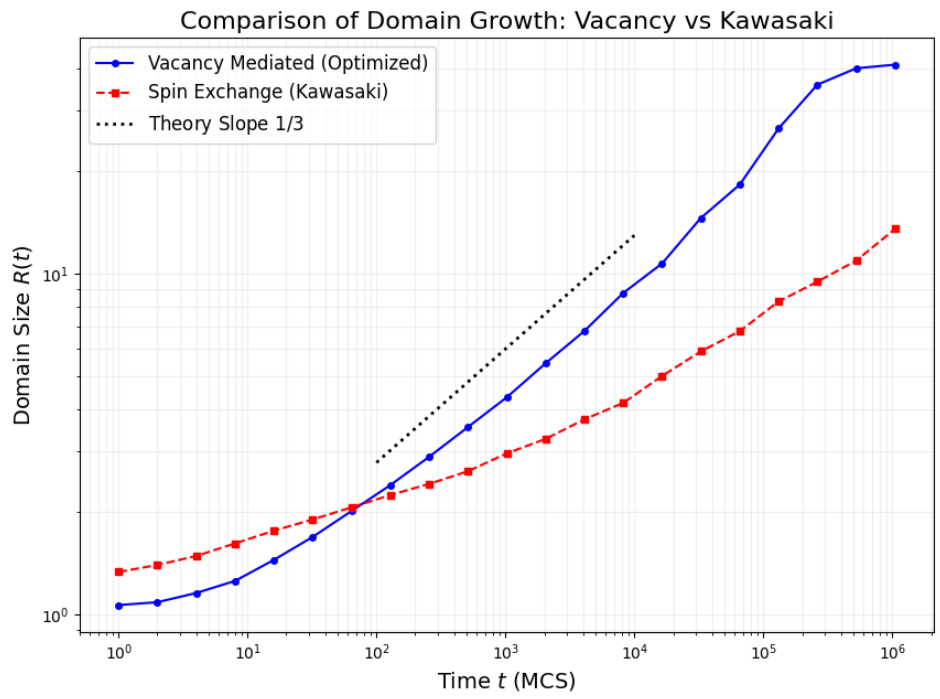
3D Simulation

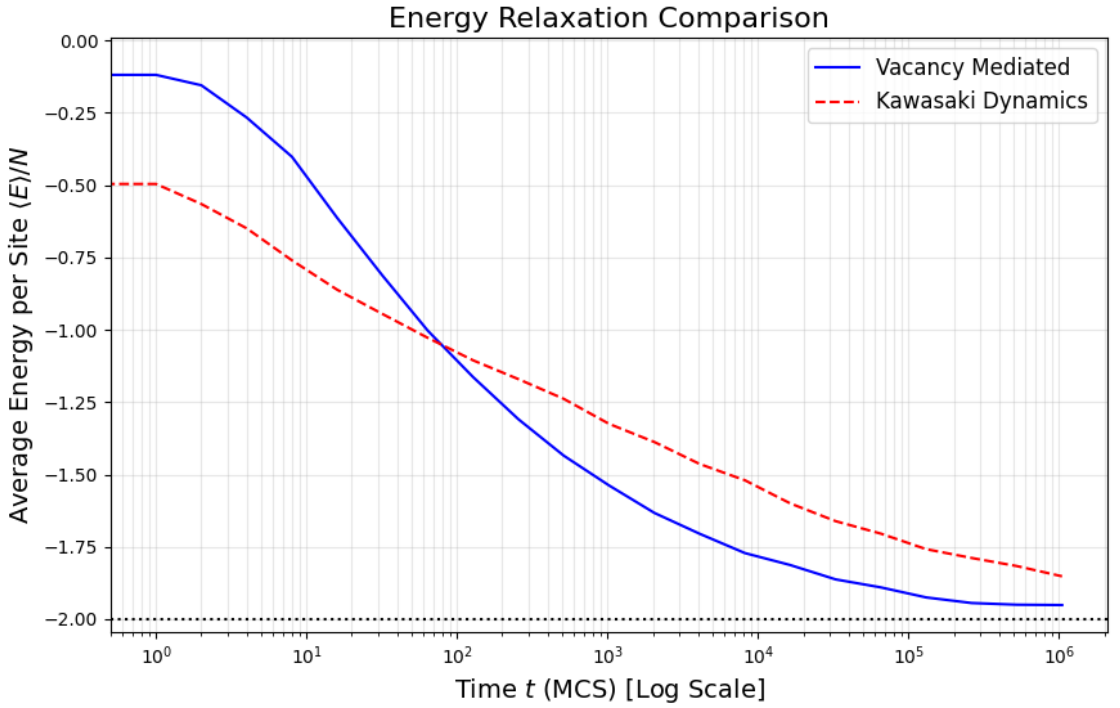


$n \approx 0.281$

Vacancy Mediated vs. Kawasaki

Evolution Efficiency: Growth & Energy

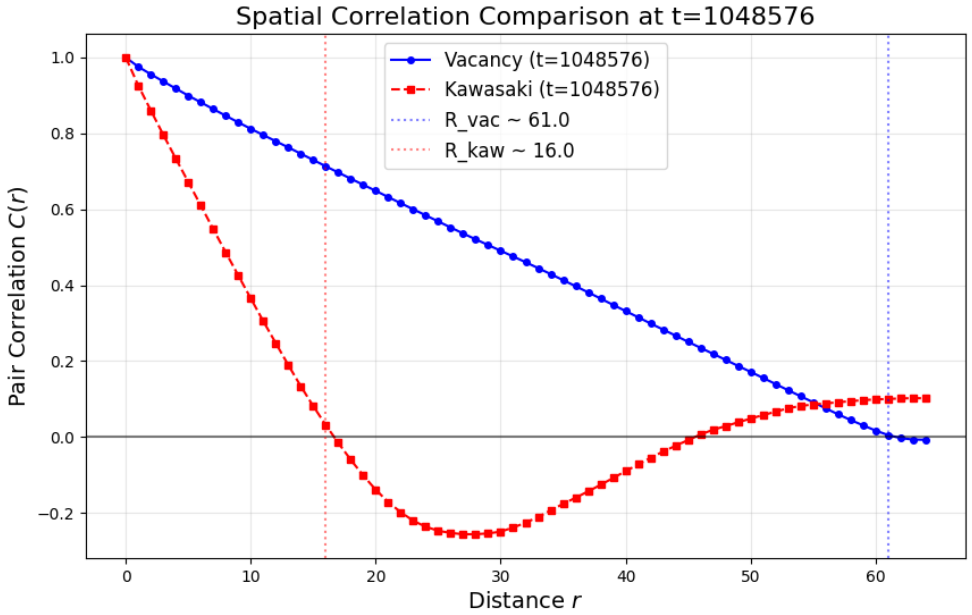


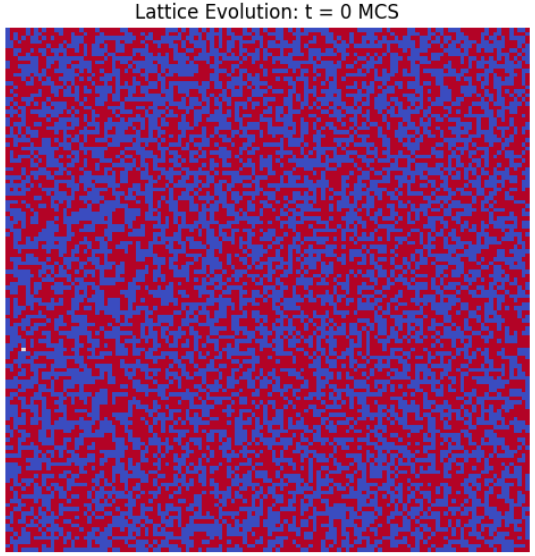


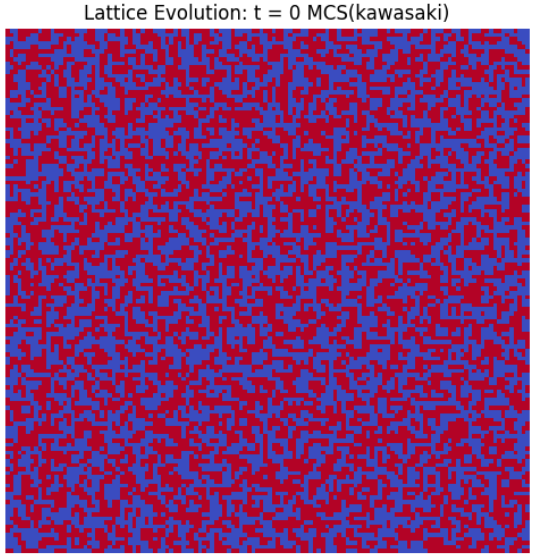
$$R_{E_{Vac}} \approx 40.96$$
$$R_{E_{kawa}} \approx 13.50$$

Vacancy Mediated vs. Kawasaki

Structural Analysis: Correlation & Morphology







Conclusion

- **Mechanism Validation**

  Validated the Vacancy-mediated Dynamics.

  Compared to Kawasaki dynamics, the physical evolution achieves greater efficiency.

- **Scaling & Saturation**

  Confirmed the Lifshitz-Slyozov Law $\left(R \sim t^{1/3}\right)$with high precision.

  Revealed **finite-size effects** (Saturation) at late stages.

- **Extended Research**

  Temperature Effects: Identified Phase Separation, Critical, and Disordered regimes.

  3D System Validation: Confirmed universality in 3D systems.

Reference

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