

Lecture5

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1 Monte Carlo: Lecture 5 Excercise

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Classical Monte Carlo simulation of a liquid–solid phase transition in a two-dimensional Lennard-Jones system

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[16]: import numpy as np
from numba import njit
import matplotlib.pyplot as plt
```

1.1 The Lennard-Jones Potential

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

1.2 The configuration Energy

$$\frac{E}{N} = \frac{2}{2} k_B T + \frac{1}{N} \left\langle \sum_{i=1}^N \sum_{i < j} U_{LJ}(r_{ij}) \right\rangle$$

```
[17]: def calculate_lennard_jones_potential(r, epsilon=1.0, sigma=1.0):
    return 4 * epsilon * ((sigma/r)**12 - (sigma/r)**6)

def calculate_energy(R:np.ndarray, T, L, epsilon=1.0, sigma=1.0):
    # First term is simply T
    total_energy = T
    # Get the sum of LJ Potentials
    N = R.shape[0]
    for j in range(N):
        rij_vec = R[j+1:] - R[j] # r_i - r_j for all i < j as differences by
        ↪vector component
        rij_vec -= np.floor(rij_vec / L + 0.5) * L # applying pbc
        rij = np.linalg.norm(rij_vec, axis=1) # calculate magnitudes as
        ↪sqrt(x**2 + y**2)
        total_energy += calculate_lennard_jones_potential(rij, epsilon, sigma).
        ↪sum()
    return total_energy
```

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def minimum_image(dr, L):
    return dr - np.floor(dr / L + 0.5) * L

def particle_energy(i, R, L, epsilon=1.0, sigma=1.0, rcut=None):
    """Sum_{j!=i} U(r_ij) with PBC"""
    dr = R - R[i]
    dr = minimum_image(dr, L)
    rij = np.linalg.norm(dr, axis=1)

    # exclude self
    rij[i] = np.inf

    if rcut is not None:
        mask = rij < rcut
        rij = rij[mask]

    return calculate_lennard_jones_potential(rij, epsilon, sigma).sum()

```

1.3 Metropolis Algorithm

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[ ]: def metropolis_algorithm(func, old_x, new_x, T):
    # Calculate weight
    f_old = func(old_x)
    f_new = func(new_x)

    w = np.exp(-(f_new - f_old) / T) if f_new != np.inf else 0

    # Generate random number and evaluate
    u = np.random.random() if w<1 else 0.

    # Accept or reject move
    if u==0. or int(w+u):
        # print(f"Accept: w:{w}, u:{u}, w+u:{w+u}")
        return new_x, f_new, 1
    else:
        # print(f"Reject: w:{w}, u:{u}, w+u:{w+u}")
        return old_x, f_old, 0

def metropolis_algorithm_local(old_R, new_R, T, L, epsilon=1.0, sigma=1.0, ↴
                                rcut=None):
    """
    Fast Metropolis using ΔE for the moved particle only.
    Returns: R_next, dE (energy change), accepted (0/1)
    """

    # find moved particle index (only one should change)
    moved = np.where(np.any(old_R != new_R, axis=1))[0]

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    if len(moved) != 1:
        raise ValueError("Expected exactly one moved particle. Use local moves.
    ↵")
    i = moved[0]

    E_old_i = particle_energy(i, old_R, L, epsilon, sigma, rcut)
    E_new_i = particle_energy(i, new_R, L, epsilon, sigma, rcut)
    dE = E_new_i - E_old_i

    if dE <= 0 or np.random.random() < np.exp(-dE / T):
        return new_R, dE, 1
    else:
        return old_R, 0.0, 0

```

1.4 Simulation

```

[ ]: # Helper Functions
def gen_intial_config(N, L, mode="random"):
    if mode == "random":
        return np.random.random((N, 2)) * L
    elif mode == "lattice": # If one wants to start in a squared lattice config
        n_side = int(np.ceil(np.sqrt(N)))
        xs = (np.arange(n_side) + 0.5) * (L / n_side)
        ys = (np.arange(n_side) + 0.5) * (L / n_side)
        grid = np.array([(x, y) for x in xs for y in ys], dtype=float)
        return grid[:N].copy()
    else:
        raise ValueError("mode must be 'random' or 'lattice'")

def move_points(R, L, a=0.1):
    N = R.shape[0]
    k = np.random.randint(N)
    disp = (2*np.random.random(2) - 1) * a

    new_R = R.copy()
    new_R[k] = (new_R[k] + disp) % L # wrap into [0, L)
    return new_R

[ ]: def run_sim(
    N, num_steps, T, delta,
    rho=0.96, epsilon=1.0, sigma=1.0,
    init_mode="random",
    burn_in=None, sample_every=50,    # sample g(r) less often
    gr_dr=0.02, compute_gr=True,
    rcut=None
):
    L = np.sqrt(N / rho)

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R = gen_intial_config(N, L, mode=init_mode)

# compute full energy ONCE at the start
E = calculate_energy(R, T=T, L=L, epsilon=epsilon, sigma=sigma)

if burn_in is None:
    burn_in = num_steps // 4

# g(r) setup
r_max = L/2
nbins = int(r_max/gr_dr)
hist = np.zeros(nbins, dtype=float)
gr_samples = 0

def accumulate_gr(config):
    nonlocal hist
    for i in range(N - 1):
        dr = config[i+1:] - config[i]
        dr -= np.floor(dr / L + 0.5) * L
        rij = np.linalg.norm(dr, axis=1)
        valid = rij < r_max
        bins = (rij[valid] / gr_dr).astype(int)
        for b in bins:
            if 0 <= b < nbins:
                hist[b] += 2

def finalize_gr(hist_avg):
    rho_here = N/(L*L)
    r = (np.arange(nbins)+0.5)*gr_dr
    shell_area = 2*np.pi*r*gr_dr
    g = (hist_avg/N)/(rho_here*shell_area)
    return r, g

accepted_total = 0
energies = []

for step in range(num_steps):
    new_R = move_points(R, L=L, a=delta) # local move

    R_next, dE, accepted = metropolis_algorithm_local(
        R, new_R, T=T, L=L, epsilon=epsilon, sigma=sigma, rcut=rcut
    )

    if accepted:
        R = R_next
        E += dE # update running energy

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        energies.append(E)
        accepted_total += accepted

        if compute_gr and step >= burn_in and (step % sample_every == 0):
            accumulate_gr(R)
            gr_samples += 1

    acc_rate = accepted_total / num_steps

    if compute_gr and gr_samples > 0:
        r, g = finalize_gr(hist / gr_samples)
    else:
        r, g = None, None

    return R, L, np.array(energies), acc_rate, r, g

```

1.5 Simulation Results

```

[ ]: N = 242
rho = 0.96
T = 0.5
num_steps = 200_000
delta = 0.08
init_mode = "lattice" # or "random"

R0, L, E_hist0, acc0, r0, g0 = run_sim(
    N=N,
    num_steps=num_steps,
    T=T,
    delta=delta,
    rho=rho,
    init_mode=init_mode,
    compute_gr=True
)

# Remove equilibration (burn-in)
burn_in = num_steps // 4
E_prod = E_hist0[burn_in:]

E_mean = np.mean(E_prod)
E_std = np.std(E_prod, ddof=1)
E_per_particle = E_mean / N

print("===== SIMULATION RESULTS REPORT =====")
print("System parameters:")
print(f" Number of particles (N): {N}")
print(f" Density (rho*): {rho}")

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print(f" Box size (L): {L:.4f}")
print(f" Temperature (T*): {T}")
print(f" Initial configuration: {init_mode}")

print("\nSimulation parameters:")
print(f" Iterations: {num_steps}")
print(f" Displacement amplitude ( $\Delta$ ): {delta}")
print(f" Acceptance rate: {acc0:.3f}")

print("\nEnergy results:")
print(f" Mean total energy: {E_mean:.6f}")
print(f" Energy standard deviation ( $\sigma_E$ ): {E_std:.6f}")
print(f" Energy per particle (E/N): {E_per_particle:.6f}")

print("\nStructure:")
if r0 is not None:
    print(" Radial distribution function g(r): computed")
else:
    print(" Radial distribution function g(r): not computed")

print("=====")  

# Plots
## Final particle positions
plt.figure(figsize=(6, 6))
plt.scatter(R0[:, 0], R0[:, 1], s=10)
plt.xlim(0, L)
plt.ylim(0, L)
plt.gca().set_aspect("equal", adjustable="box")
plt.title("Final particle positions")
plt.xlabel("x")
plt.ylabel("y")
plt.tight_layout()
plt.show()

# Energy vs Monte Carlo steps
steps = np.arange(len(E_hist0))

burn_in = len(E_hist0) // 4

plt.figure(figsize=(7, 4))
plt.plot(steps, E_hist0, linewidth=1)
plt.title("Energy vs Monte Carlo steps")
plt.xlabel("MC step")
plt.ylabel("Energy")
plt.tight_layout()
plt.show()

```

===== MONTE CARLO LENNARD-JONES REPORT =====

System parameters:

Number of particles (N): 242
Density (ρ^*): 0.96
Box size (L): 15.8771
Temperature (T *): 0.5
Initial configuration: lattice

Simulation parameters:

Iterations: 200000
Displacement amplitude (Δ): 0.08
Acceptance rate: 0.394

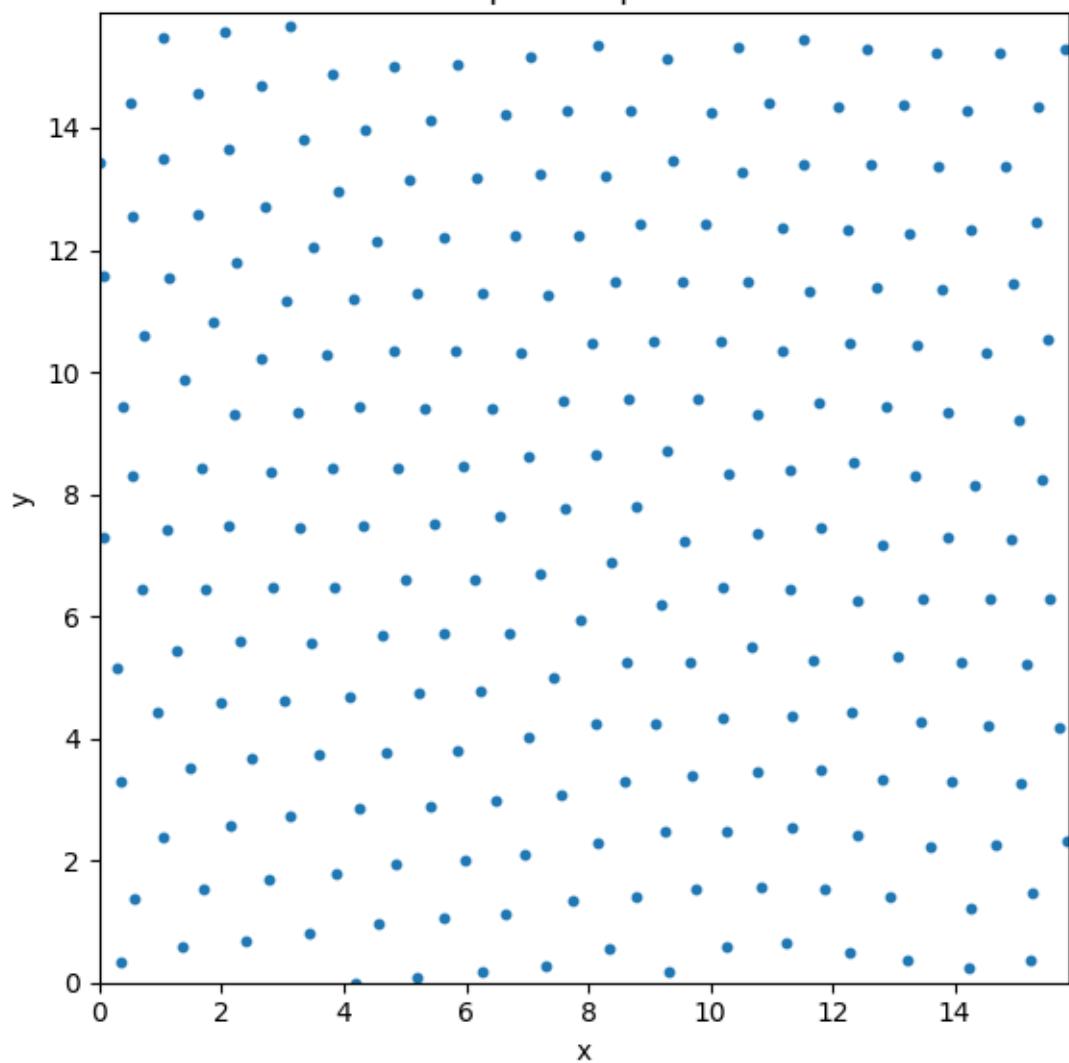
Energy results:

Mean total energy: -623.120505
Energy standard deviation (σ_E): 28.774889
Energy per particle (E/N): -2.574878

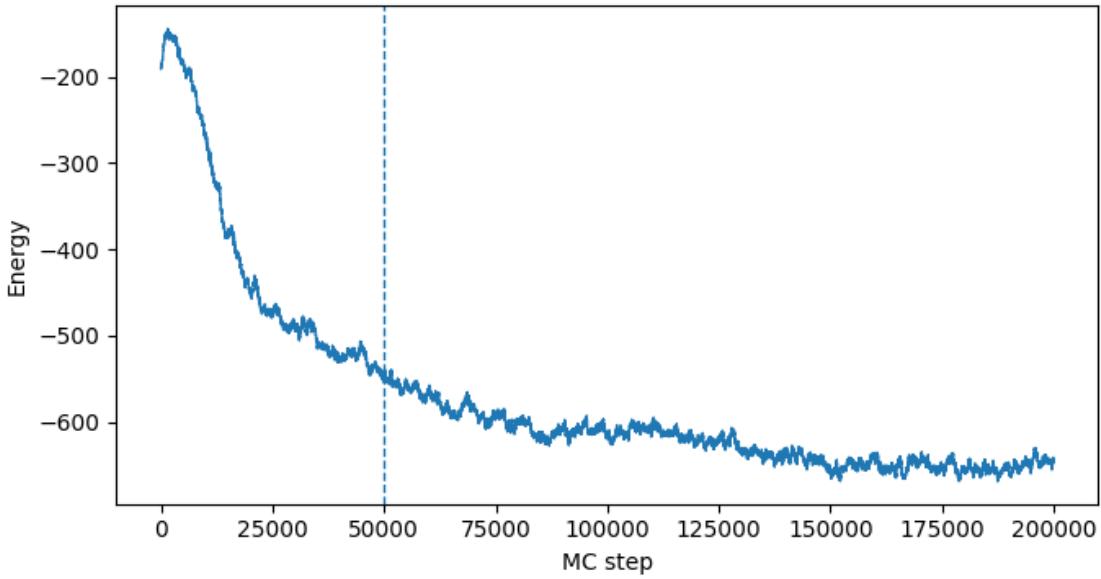
Structure:

Radial distribution function $g(r)$: computed

Final particle positions



Energy vs Monte Carlo steps



```
[ ]: # RUN ALL TEMPERATURES
N = 242
rho = 0.96
num_steps = 200_000
init_mode = "lattice"
temps = [0.5, 1.0, 1.5, 2.0, 2.5, 3.0]
delta_default = 0.08
delta_by_T = {T: delta_default for T in temps}
burn_in = num_steps // 4
sigma = 1.0

results = []

for T in temps:
    delta = delta_by_T[T]

    R, L, E_hist, acc, r, g = run_sim(
        N=N,
        num_steps=num_steps,
        T=T,
        delta=delta,
        rho=rho,
        init_mode=init_mode,
        compute_gr=True
    )
```

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# production window
E_prod = E_hist[burn_in:]
E_mean = np.mean(E_prod)
E_std = np.std(E_prod, ddof=1)

E_sem = E_std / np.sqrt(len(E_prod))

results.append({
    "T": T,
    "delta": delta,
    "acc": acc,
    "L": L,
    "R": R,
    "E_hist": E_hist,
    "E_mean": E_mean,
    "E_std": E_std,
    "E_sem": E_sem,
    "E_per_particle": E_mean / N,
    "EperN_sem": E_sem / N,
    "r": r,
    "g": g
})

# PRINT REPORT TABLE
print("===== SIMULATION RESULTS REPORT =====")
print(f"System: N={N}, rho*={rho}, init_mode={init_mode}")
print("-----")
print(" T*      steps      Δ      acc      <E>/N      err(E/N)")
print("-----")
for res in results:
    print(f"{res['T']:4.1f} {res['num_steps']:7d} {res['delta']:5.3f} {res['acc']:6.
        ↵3f} "
          f"{res['E_per_particle']:10.6f} {res['EperN_sem']:10.6f}")
print("-----")
print("Note: err(E/N) here is std/sqrt(M) (naive; MC samples are correlated).")
print("=====")
# SNAPSHOTS: crystal vs gas
def plot_snapshot(R, L, title):
    plt.figure(figsize=(6, 6))
    plt.scatter(R[:, 0], R[:, 1], s=10)
    plt.xlim(0, L); plt.ylim(0, L)
    plt.gca().set_aspect("equal", adjustable="box")
    plt.title(title)
    plt.xlabel("x"); plt.ylabel("y")
    plt.tight_layout()

```

```

plt.show()

# crystal-like: lowest T, gas-like: highest T
plot_snapshot(results[0]["R"], results[0]["L"], f"Snapshot (crystal-like)_{T*={results[0]['T']}\"})
plot_snapshot(results[-1]["R"], results[-1]["L"], f"Snapshot (gas-like)_{T*={results[-1]['T']}\")

# ENERGY vs MC steps (show for low & high T)
def plot_energy_trace(E_hist, T):
    plt.figure(figsize=(7, 4))
    plt.plot(np.arange(len(E_hist)), E_hist, linewidth=1)
    plt.axvline(burn_in, linestyle="--", linewidth=1)
    plt.title(f"Energy vs Monte Carlo steps (T*={T})")
    plt.xlabel("MC step")
    plt.ylabel("Energy")
    plt.tight_layout()
    plt.show()

plot_energy_trace(results[0]["E_hist"], results[0]["T"])
plot_energy_trace(results[-1]["E_hist"], results[-1]["T"])

# E/N vs T with error bars
Tvals = np.array([r["T"] for r in results])
EperN = np.array([r["E_per_particle"] for r in results])
EperN_err = np.array([r["EperN_sem"] for r in results])

plt.figure(figsize=(6,4))
plt.errorbar(Tvals, EperN, yerr=EperN_err, fmt='o-', capsize=3)
plt.title("Energy per particle vs temperature")
plt.xlabel("T*")
plt.ylabel("E/N")
plt.tight_layout()
plt.show()

# g(r) vs r/sigma (all temperatures)
plt.figure(figsize=(6,4))
for res in results:
    if res["r"] is None or res["g"] is None:
        continue
    plt.plot(res["r"] / sigma, res["g"], label=f"T*={res['T']}\")
plt.title("Radial distribution function")
plt.xlabel(r"$r/\sigma$")
plt.ylabel("g(r)")
plt.legend()
plt.tight_layout()
plt.show()

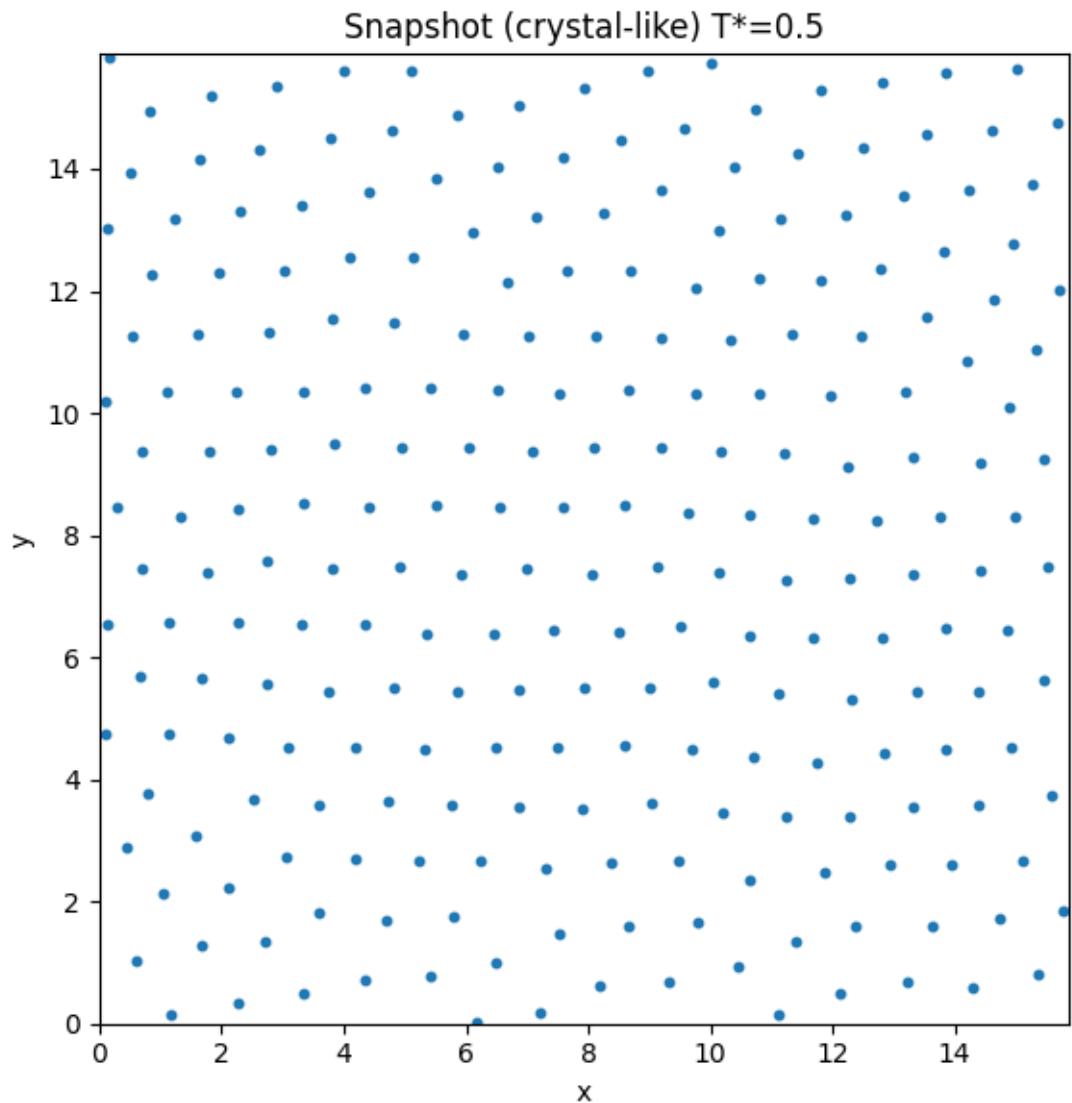
```

===== SIMULATION RESULTS REPORT =====

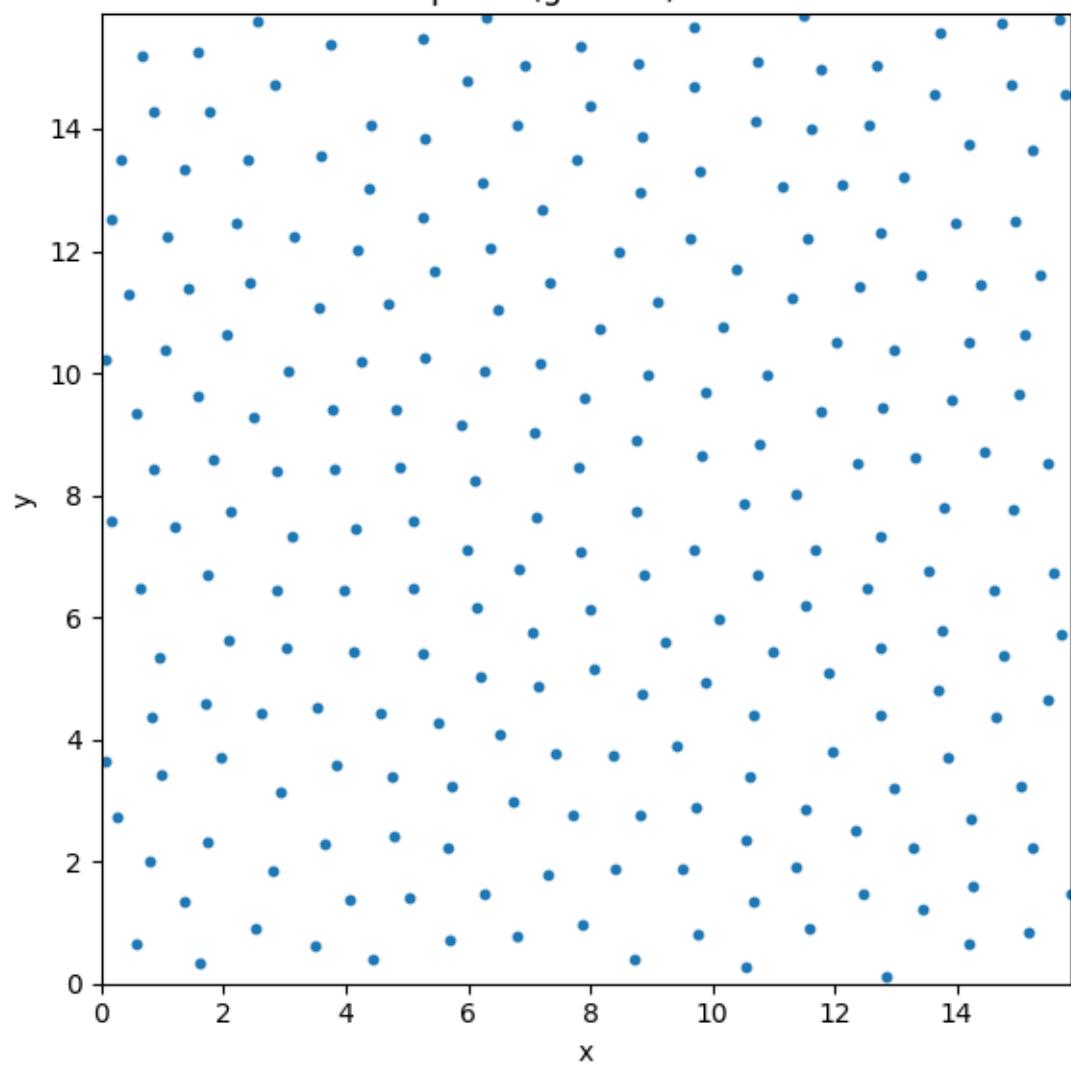
System: N=242, rho*=0.96, init_mode=lattice

T*	steps	Δ	acc	$\langle E \rangle / N$	err(E/N)
0.5	200000	0.080	0.398	-2.613762	0.000200
1.0	200000	0.080	0.503	-2.103227	0.000314
1.5	200000	0.080	0.551	-1.575244	0.000211
2.0	200000	0.080	0.584	-1.168282	0.000300
2.5	200000	0.080	0.607	-0.708810	0.000369
3.0	200000	0.080	0.628	-0.433216	0.000450

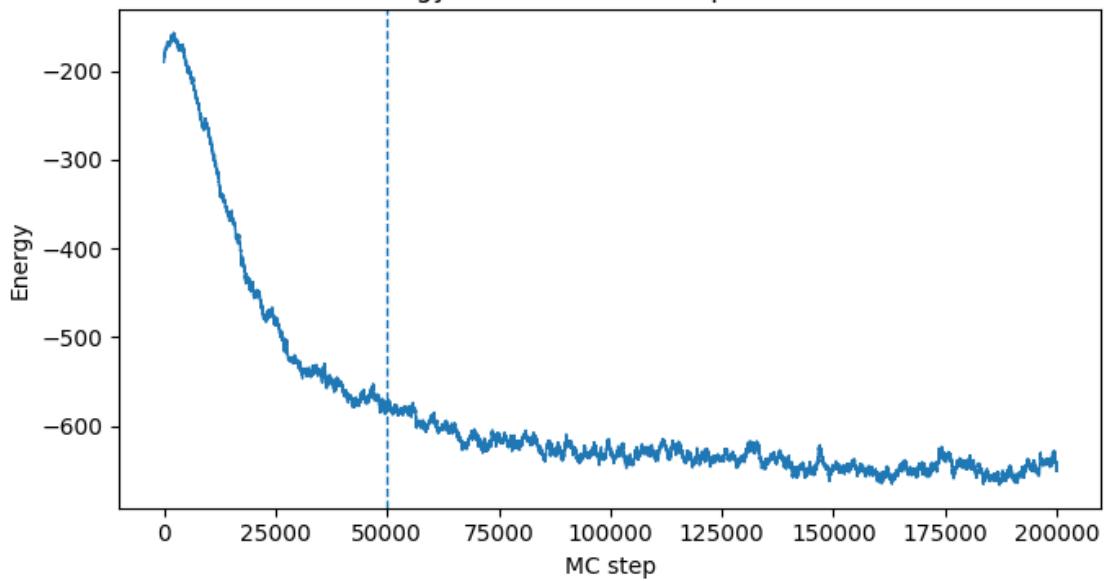
Note: err(E/N) here is std/sqrt(M) (naive; MC samples are correlated).



Snapshot (gas-like) $T^*=3.0$



Energy vs Monte Carlo steps ($T^*=0.5$)



Energy vs Monte Carlo steps ($T^*=3.0$)

