Freie Universität Berlin

Computational Sciences Projektseminar

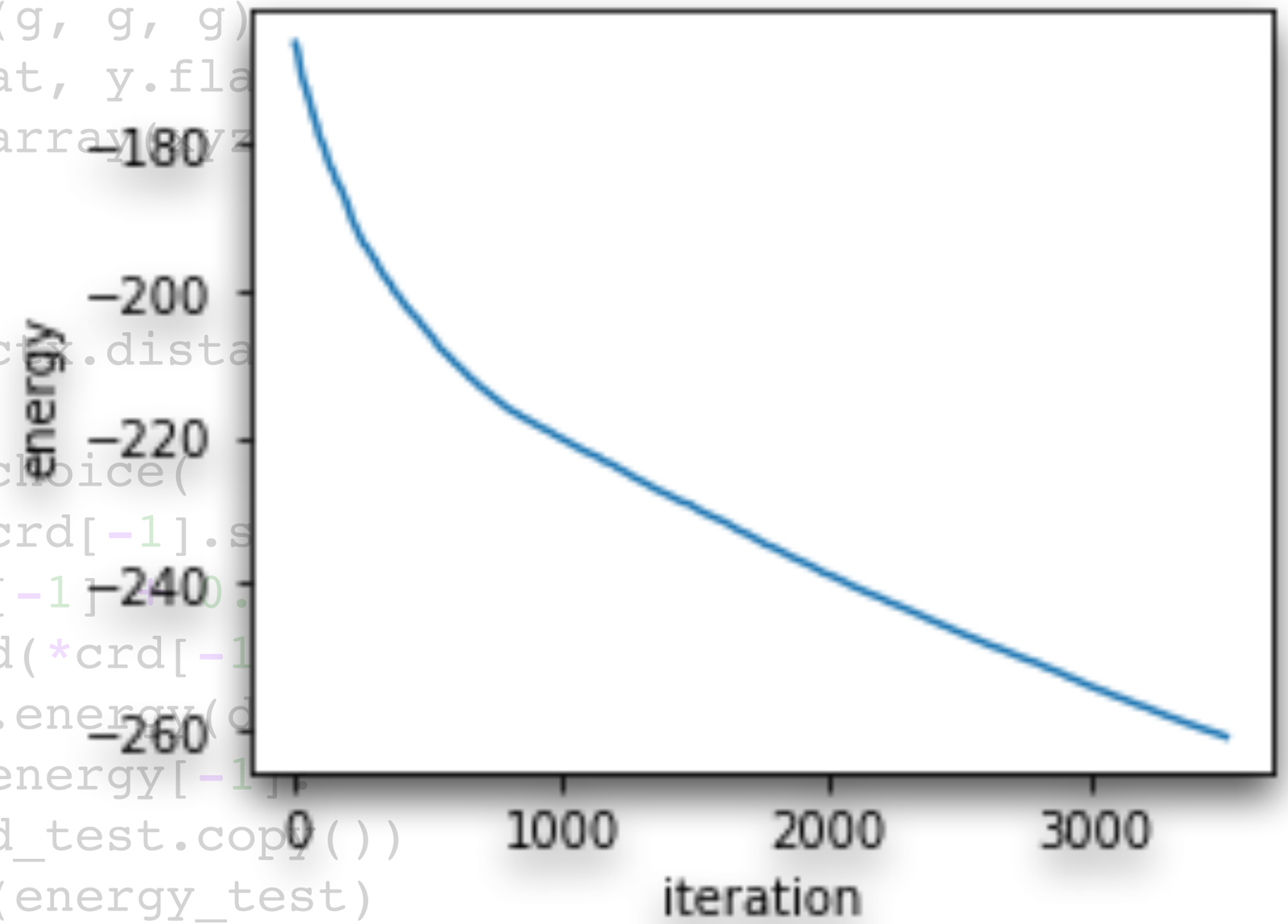
Simulating a periodic box with a Lennard-Jones fluid

The test system

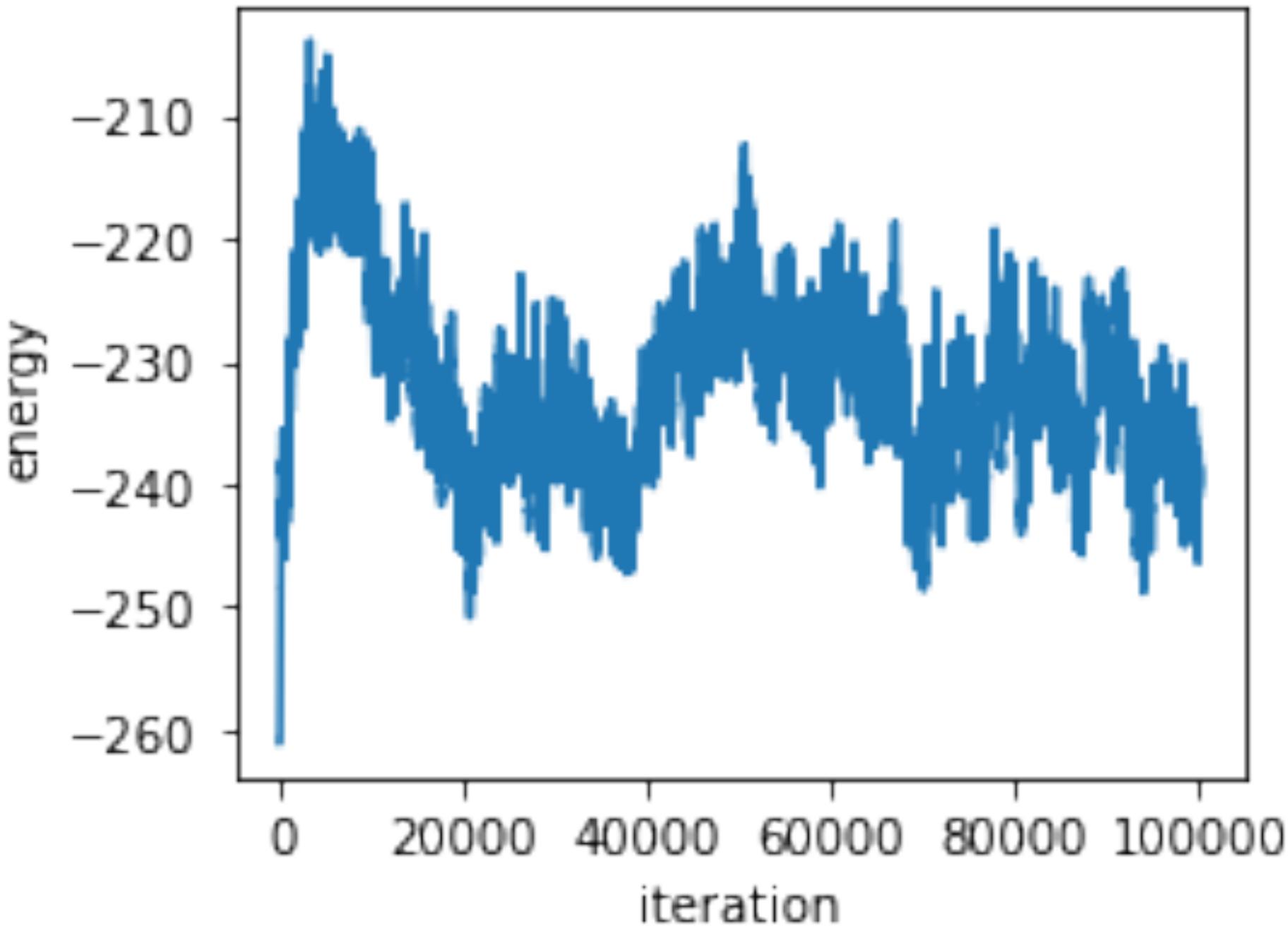
- Lennard-Jones only, no Coulomb/Ewald
- 64 particles in a periodic/cubic box of length 5
- use parameters $\varepsilon = \sigma = 1$ for every particle
- use a cutoff of $r_{cut} = 2.5$ for neighbour lists

Initial structure and optimisation

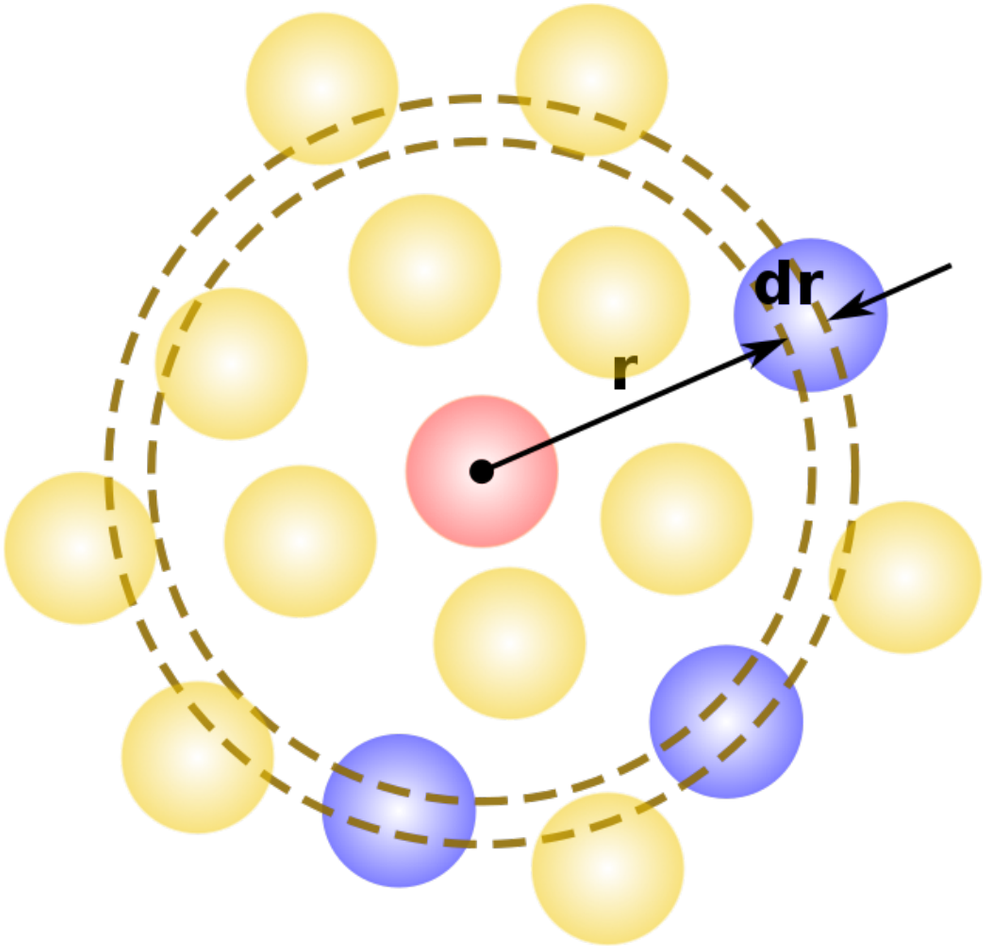
```
g = [0, 1, 2, 3]
x, y, z = np.meshgrid(g, g, g)
xyz = np.vstack((x.flat, y.fla
xyz = np.ascontiguousarray(xyz


crd = [xyz.copy()]
energy = [vdw.energy(crd[-1].dista
for _ in range(1000):
    mask = np.random.choice(
        [0, 1], size=crd[-1].s
    crd_test[:] = crd[-1] + 0.
        np.random.rand(*crd[-1
    energy_test = vdw.energy(c
    if energy_test < energy[-1]:
        crd.append(crd_test.copy())
        energy.append(energy_test)
```

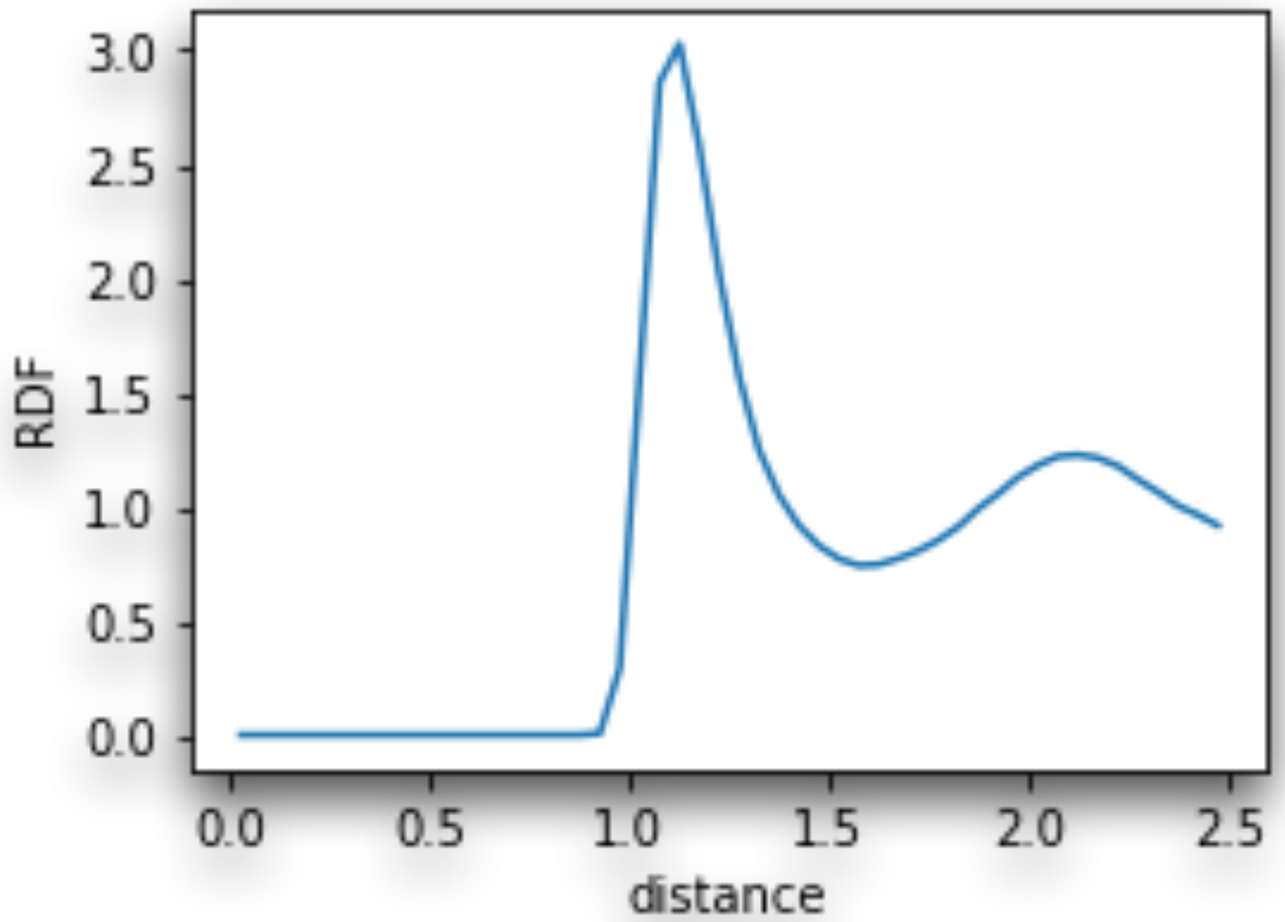


Simulation via Metropolis MC



Pair correlation function





$$g(r) = \frac{\langle \#\text{ of neighbours at distance } r \rangle}{\langle \#\text{ of ideal gas particles at distance } r \rangle}$$