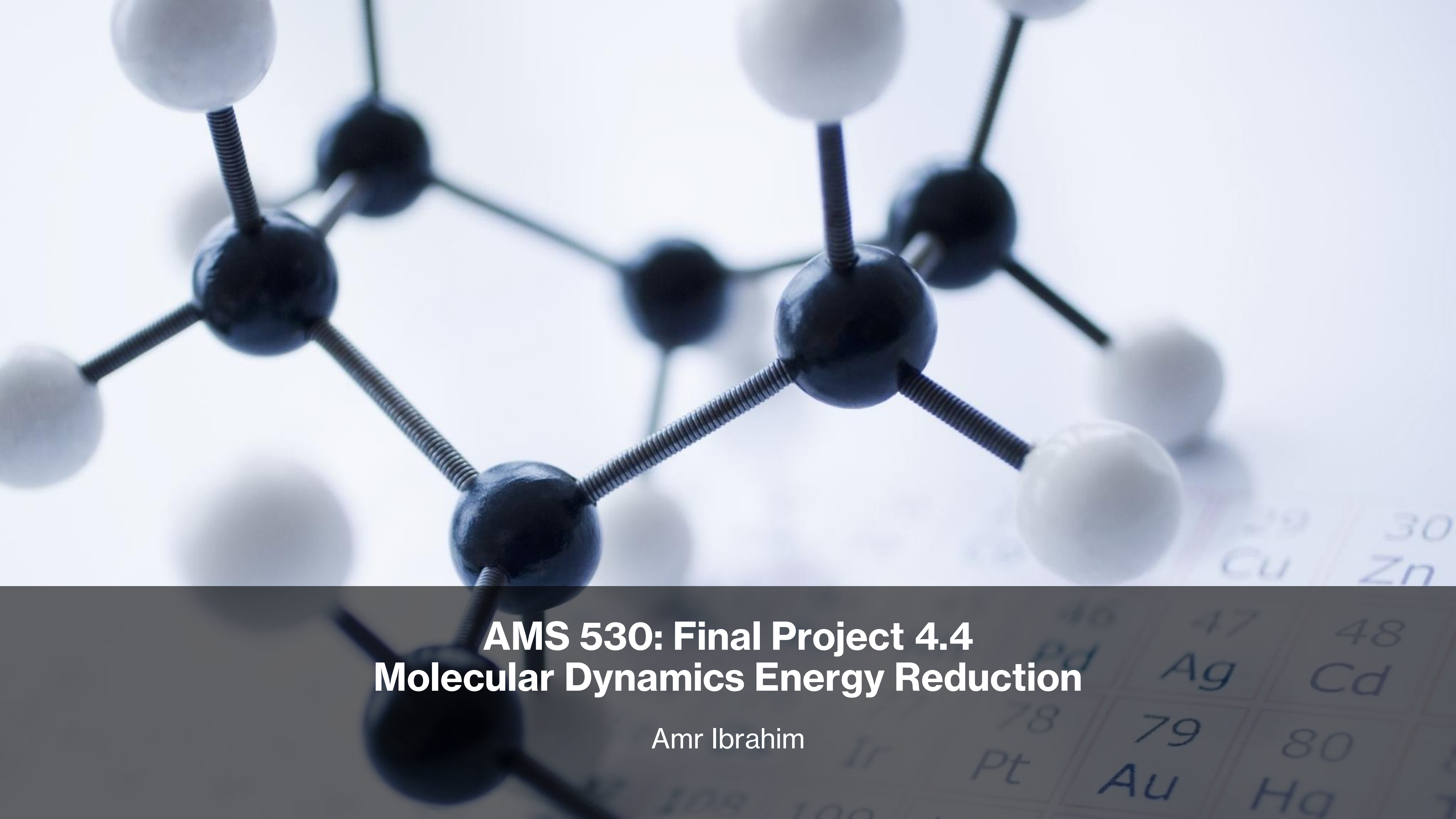

AMS 530: Final Project 4.4
Molecular Dynamics Energy Reduction

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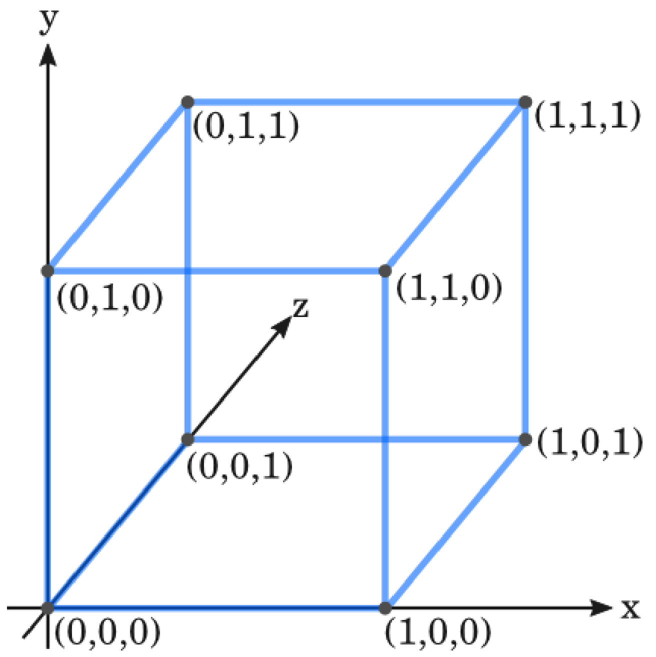
Problem Statement

- Goal: Reduce energy of given system of particles by kicking them around
  - Emphasis on parallelization of energy reduction
- Total Energy is given by
  - $\frac{1}{2}\sum_{j\neq i}^{N} V_{ij}$
  - Lenard-Jones potential (ignoring constants)
    - $V_{ij} = \frac{1}{r_{ij}^{12}} - \frac{2}{r_{ij}^{6}}$
    - $r_{ij} = |x_i - x_j|$
- Initial conditions:
  - Box 10x10x10
  - N = 11x11x11 particles placed at box grid points

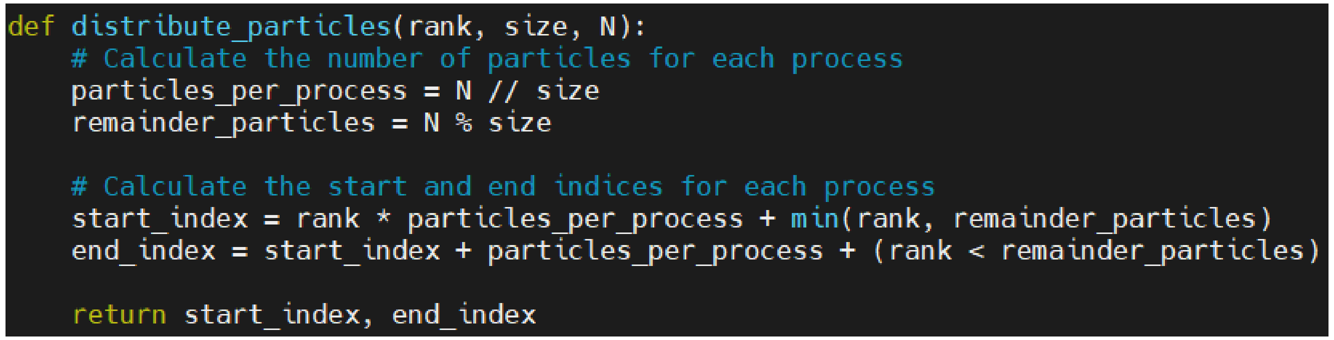


Program: General Design

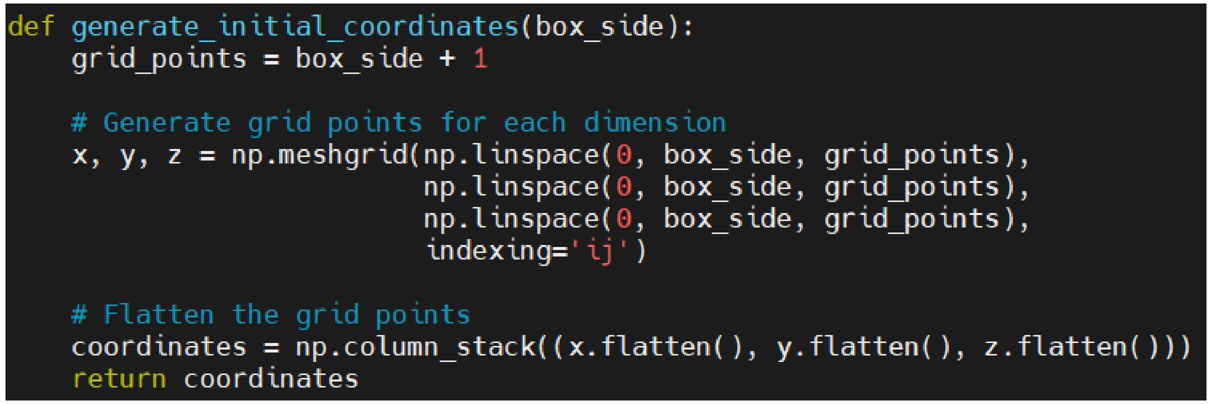
1. Generate initial coordinates & initial energy E_0
   - Initial coordinates generated by all processes
   - Particles distributed among processes
   - Energy calculation
2. Move a particle randomly with max distance 0.5
   - Moving a fraction of particles at a time
   - Discard moves that do not reduce energy
   - If particle moves outside the box return it from the opposite side
3. Repeat step 2 for 100 steps and print out energy if lowered

Program

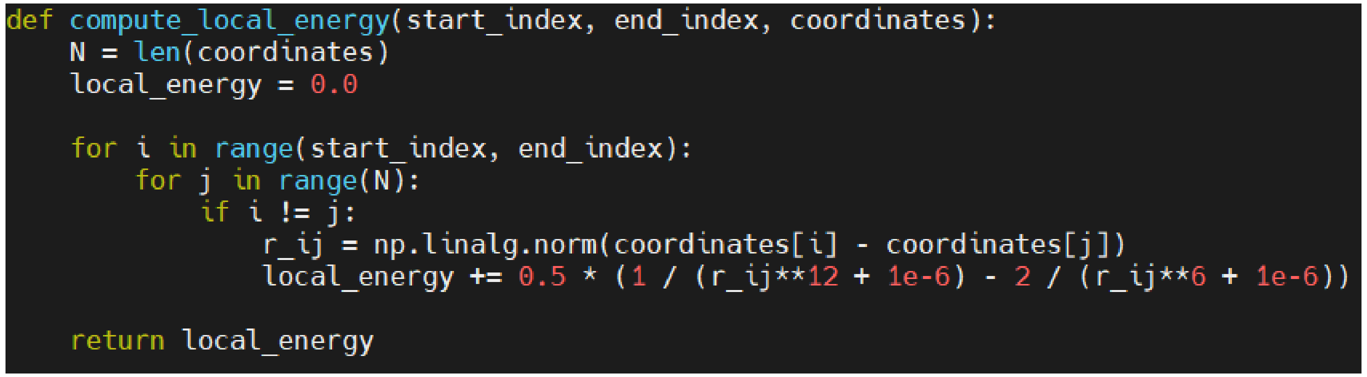
- Distribute particles
  - Based on N // size
  - Add remainder particles evenly across processes
- Generate initial coordinates
  - For all processes
  - All processes require full coordinates to compute initial energy
- Compute local energy
  - Compute interactions of local particles
  - Total energy = $\sum_{i=0}^{P} local\ energy_i$



```python
def distribute_particles(rank, size, N):
    # Calculate the number of particles for each process
    particles_per_process = N // size
    remainder_particles = N % size

    # Calculate the start and end indices for each process
    start_index = rank * particles_per_process + min(rank, remainder_particles)
    end_index = start_index + particles_per_process + (rank < remainder_particles)

    return start_index, end_index
```

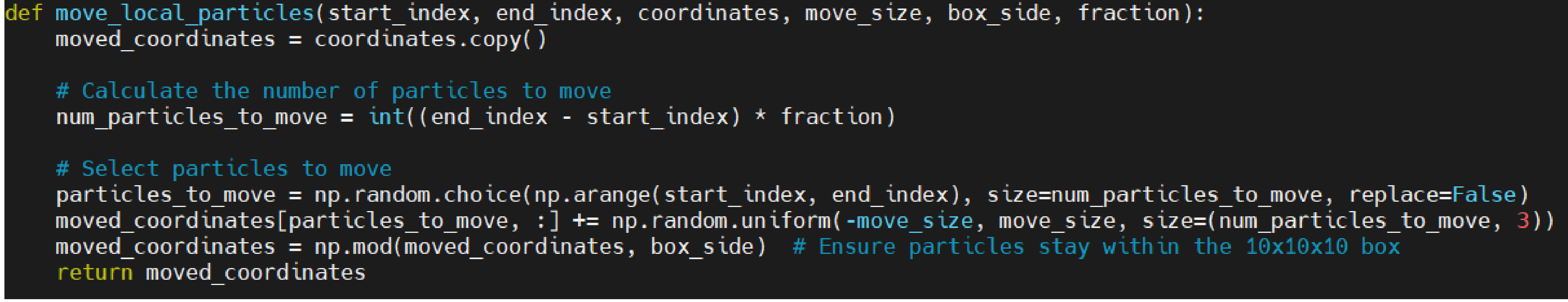


```python
def generate_initial_coordinates(box_side):
    grid_points = box_side + 1

    # Generate grid points for each dimension
    x, y, z = np.meshgrid(np.linspace(0, box_side, grid_points),
                          np.linspace(0, box_side, grid_points),
                          np.linspace(0, box_side, grid_points),
                          indexing='ij')

    # Flatten the grid points
    coordinates = np.column_stack((x.flatten(), y.flatten(), z.flatten()))
    return coordinates
```



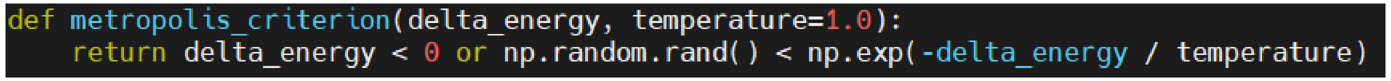
```python
def compute_local_energy(start_index, end_index, coordinates):
    N = len(coordinates)
    local_energy = 0.0

    for i in range(start_index, end_index):
        for j in range(N):
            if i != j:
                r_ij = np.linalg.norm(coordinates[i] - coordinates[j])
                local_energy += 0.5 * (1 / (r_ij**12 + 1e-6) - 2 / (r_ij**6 + 1e-6))

    return local_energy
```

Program



```python
def move_local_particles(start_index, end_index, coordinates, move_size, box_side, fraction):
    moved_coordinates = coordinates.copy()

    # Calculate the number of particles to move
    num_particles_to_move = int((end_index - start_index) * fraction)

    # Select particles to move
    particles_to_move = np.random.choice(np.arange(start_index, end_index), size=num_particles_to_move, replace=False)
    moved_coordinates[particles_to_move, :] += np.random.uniform(-move_size, move_size, size=(num_particles_to_move, 3))
    moved_coordinates = np.mod(moved_coordinates, box_side)  # Ensure particles stay within the 10x10x10 box
    return moved_coordinates
```

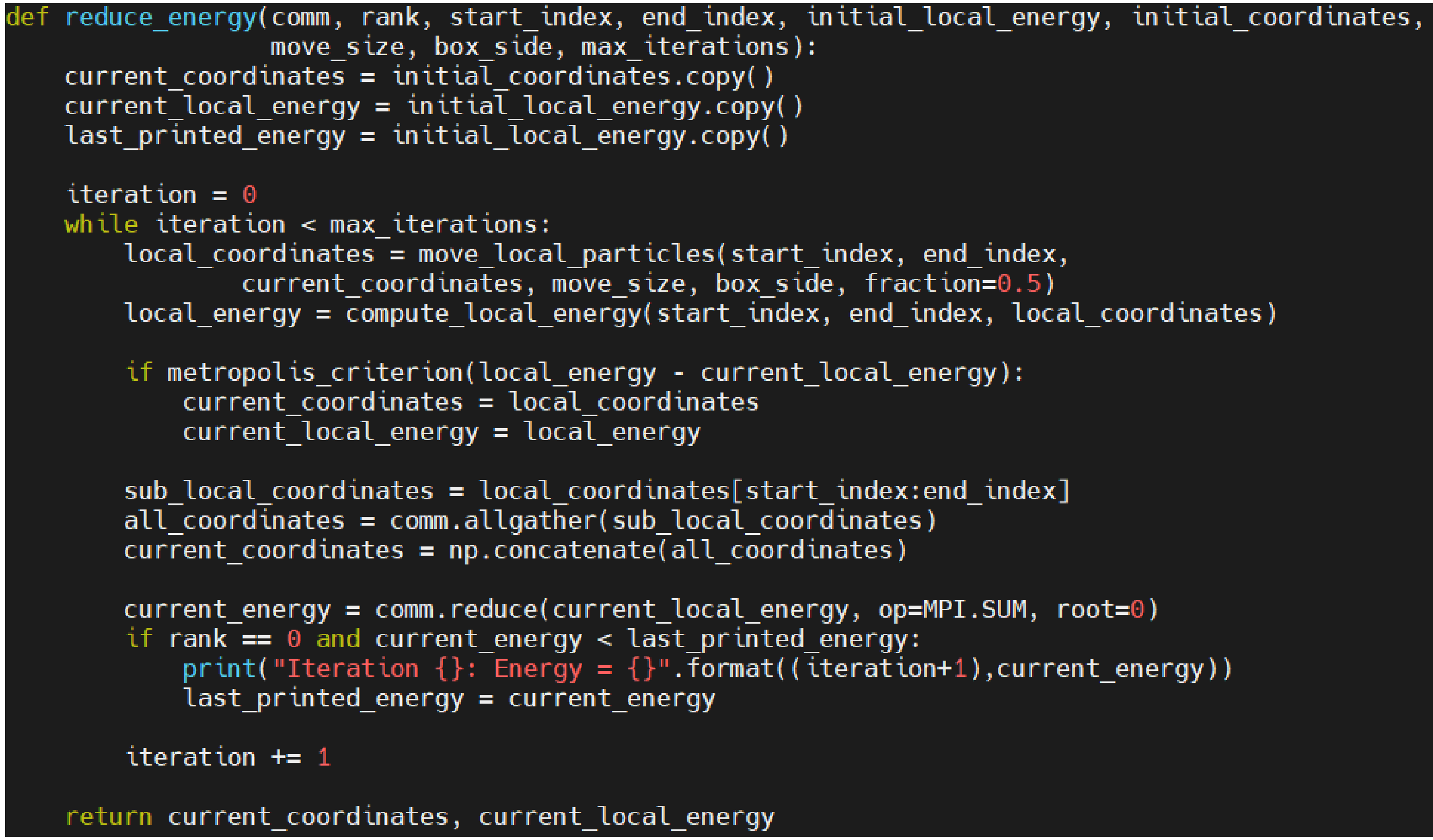
- Move local particles
  - Move a fraction of randomly chosen particles
  - Move with distribution U(-0.5, 0.5)
  - Mod coordinates
- Metropolis criterion (Simulated Annealing)
  - Update local coordinates & local energy if
    - $E_{local_i} - E_{local_0} < 0$
    - $rand < e^{-(E_{local_i} - E_{local_0})/T}, T = 1$
  - In case stuck at local min



```python
def metropolis_criterion(delta_energy, temperature=1.0):
    return delta_energy < 0 or np.random.rand() < np.exp(-delta_energy / temperature)
```

Program

- Reduce energy
  - Move particles
  - Compute local energy
  - Metropolis criterion
  - Extract new local coordinates
    - Each process get their respective local particle coordinates
  - All gather new coordinates
    - Updated coordinates for *next iteration*
  - Compute new total energy
    - New total energy = $\sum_{i=0}^{P} local\ energy_i$



```python
def reduce_energy(comm, rank, start_index, end_index, initial_local_energy, initial_coordinates,
                  move_size, box_side, max_iterations):
    current_coordinates = initial_coordinates.copy()
    current_local_energy = initial_local_energy.copy()
    last_printed_energy = initial_local_energy.copy()

    iteration = 0
    while iteration < max_iterations:
        local_coordinates = move_local_particles(start_index, end_index,
                current_coordinates, move_size, box_side, fraction=0.5)
        local_energy = compute_local_energy(start_index, end_index, local_coordinates)

        if metropolis_criterion(local_energy - current_local_energy):
            current_coordinates = local_coordinates
            current_local_energy = local_energy

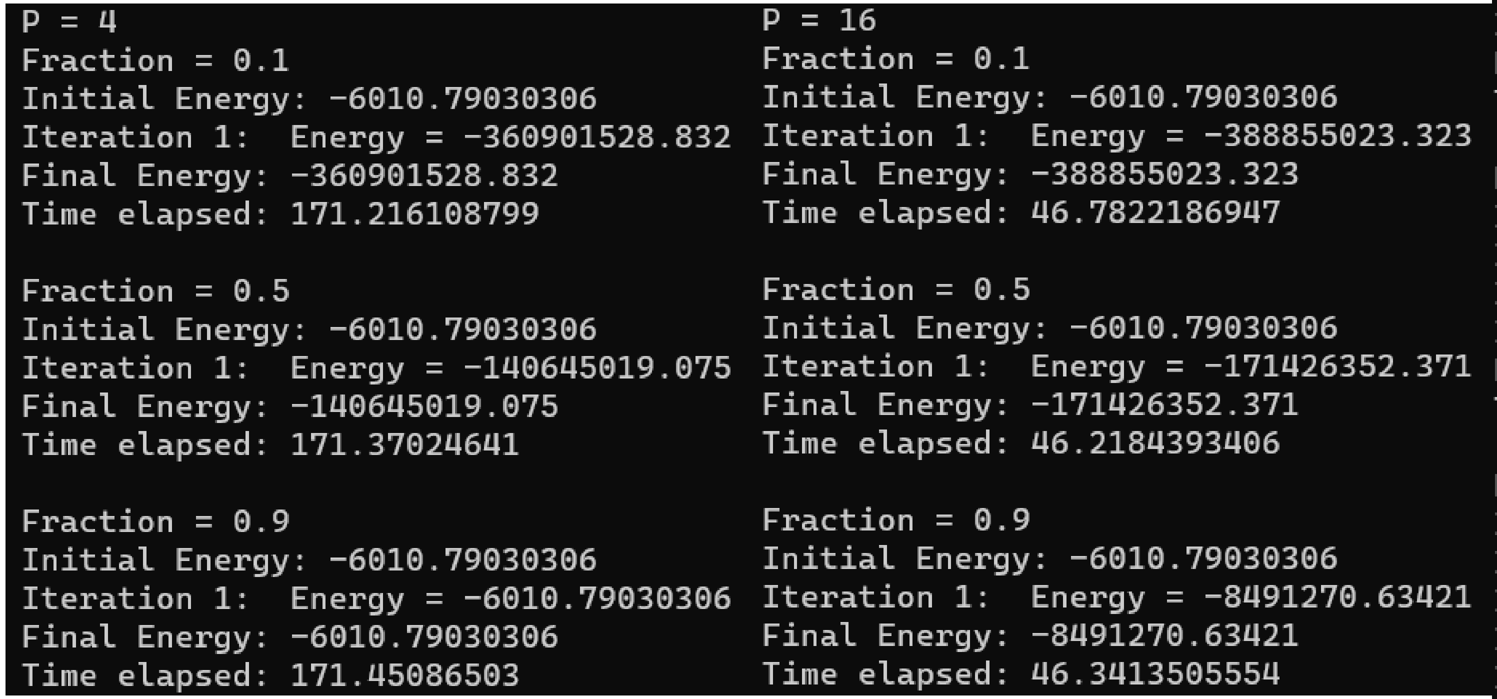
        sub_local_coordinates = local_coordinates[start_index:end_index]
        all_coordinates = comm.allgather(sub_local_coordinates)
        current_coordinates = np.concatenate(all_coordinates)

        current_energy = comm.reduce(current_local_energy, op=MPI.SUM, root=0)
        if rank == 0 and current_energy < last_printed_energy:
            print("Iteration {}: Energy = {}".format((iteration+1),current_energy))
            last_printed_energy = current_energy

        iteration += 1

    return current_coordinates, current_local_energy
```

Results



```
P = 4
Fraction = 0.1
Initial Energy: -6010.79030306
Iteration 1:  Energy = -360901528.832
Final Energy: -360901528.832
Time elapsed: 171.216108799

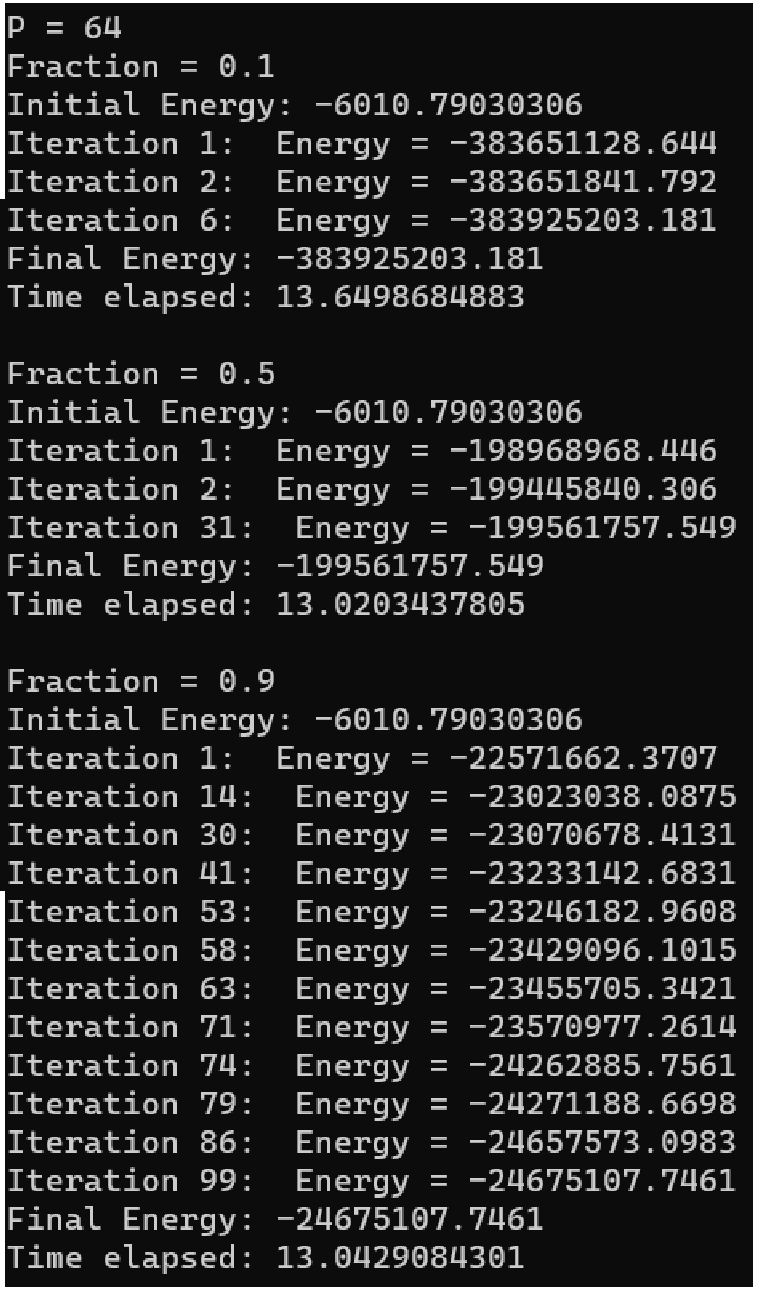
Fraction = 0.5
Initial Energy: -6010.79030306
Iteration 1:  Energy = -140645019.075
Final Energy: -140645019.075
Time elapsed: 171.37024641

Fraction = 0.9
Initial Energy: -6010.79030306
Iteration 1:  Energy = -6010.79030306
Final Energy: -6010.79030306
Time elapsed: 171.45086503
```

```
P = 16
Fraction = 0.1
Initial Energy: -6010.79030306
Iteration 1:  Energy = -388855023.323
Final Energy: -388855023.323
Time elapsed: 46.7822186947

Fraction = 0.5
Initial Energy: -6010.79030306
Iteration 1:  Energy = -171426352.371
Final Energy: -171426352.371
Time elapsed: 46.2184393406

Fraction = 0.9
Initial Energy: -6010.79030306
Iteration 1:  Energy = -8491270.63421
Final Energy: -8491270.63421
Time elapsed: 46.3413505554
```



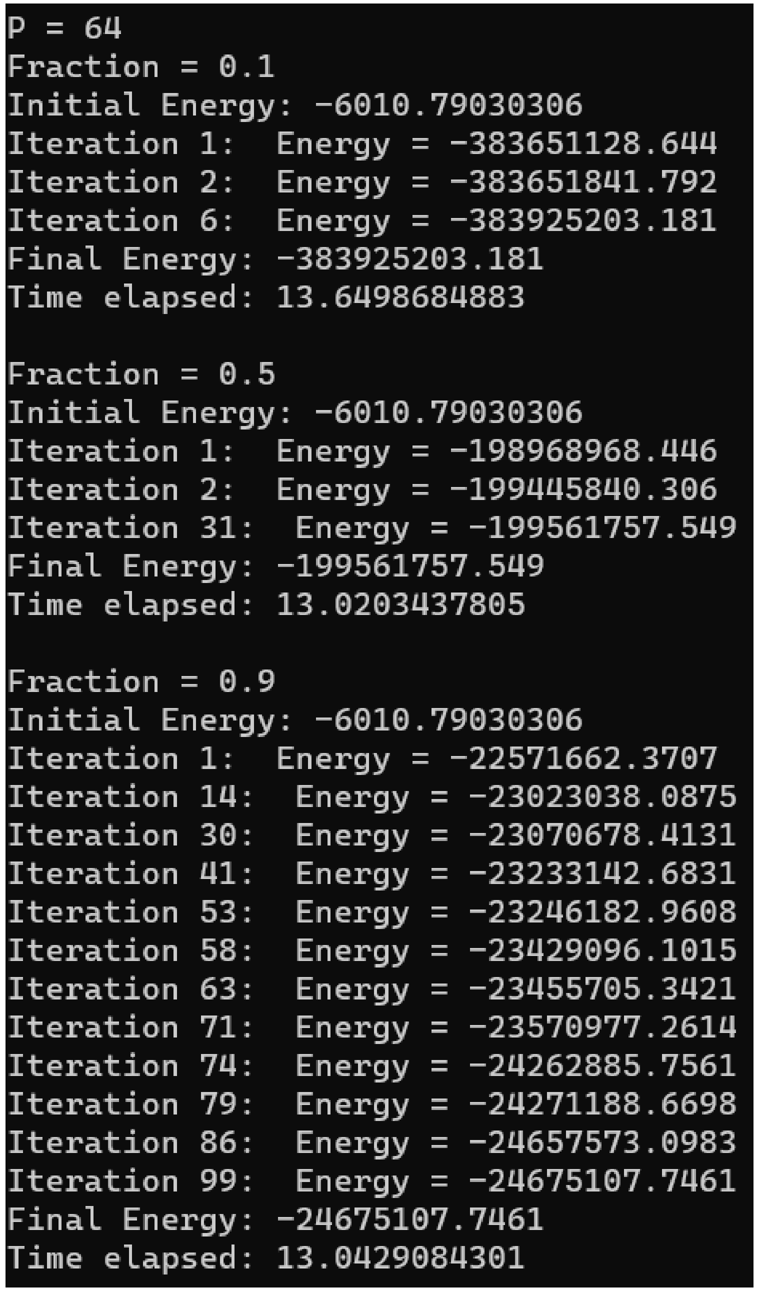
```
P = 64
Fraction = 0.1
Initial Energy: -6010.79030306
Iteration 1:  Energy = -383651128.644
Iteration 2:  Energy = -383651841.792
Iteration 6:  Energy = -383925203.181
Final Energy: -383925203.181
Time elapsed: 13.6498684883

Fraction = 0.5
Initial Energy: -6010.79030306
Iteration 1:  Energy = -198968968.446
Iteration 2:  Energy = -199445840.306
Iteration 31:  Energy = -199561757.549
Final Energy: -199561757.549
Time elapsed: 13.0203437805

Fraction = 0.9
Initial Energy: -6010.79030306
Iteration 1:  Energy = -22571662.3707
Iteration 14:  Energy = -23023038.0875
Iteration 30:  Energy = -23070678.4131
Iteration 41:  Energy = -23233142.6831
Iteration 53:  Energy = -23246182.9608
Iteration 58:  Energy = -23429096.1015
Iteration 63:  Energy = -23455705.3421
Iteration 71:  Energy = -23570977.2614
Iteration 74:  Energy = -24262885.7561
Iteration 79:  Energy = -24271188.6698
Iteration 86:  Energy = -24657573.0983
Iteration 99:  Energy = -24675107.7461
Final Energy: -24675107.7461
Time elapsed: 13.0429084301
```

Discussion

- Energy reduction
  - 1st step usually has a massive reduction
  - As fraction number increases reduction of energy is reduced
  - Among iterations reduction is small compared to 1st iteration
- Time elapsed
  - Within each P, time elapsed variance is very small
  - As P increases time elapsed decreases



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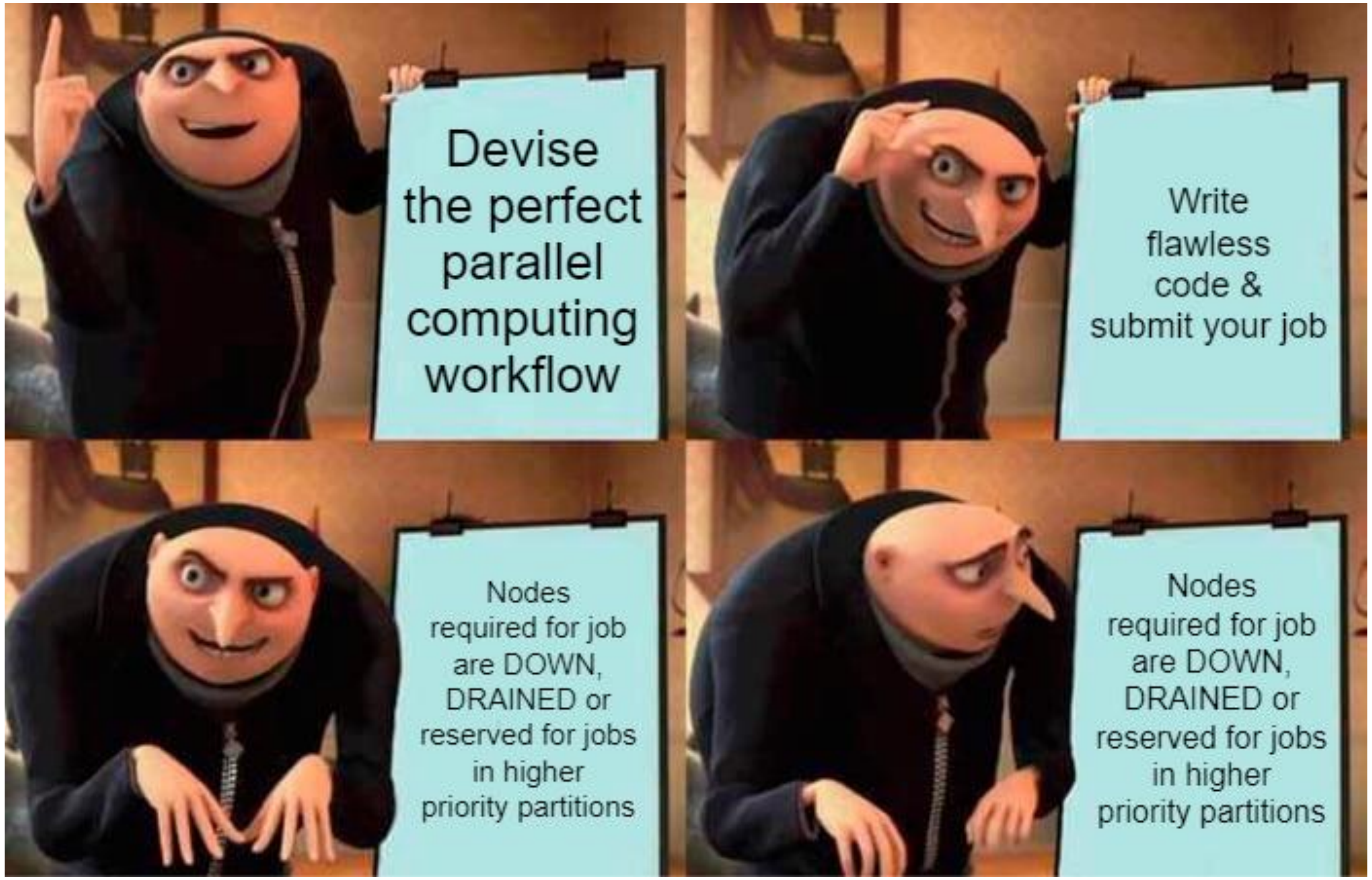
Time elapsed: 13.0429084301
```

Future Direction

- Decomposition
  - This project uses particle decomposition
  - Spatial + particle decomposition
- Energy reduction
  - Method applied Monte Carlo
  - Gradient descent
  - Python’s scipy.optimize()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