Metropolis Algorithm

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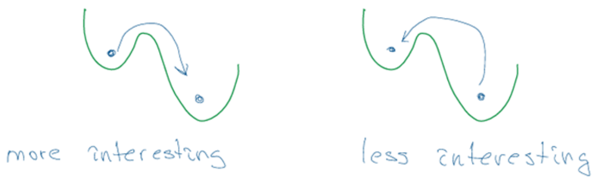
Introduction

Using importance sampling it is possible to decrease the variance in estimation of the value of an integral. We consider the following problem of optimisation: finding the global optimum of a given function. Generally, the function can have a larger number of variables/degrees of freedom and an Newton steepest descent method can be inefficient as the number of local minimum can be large. A better efficiency can be obtained if the jump over barriers is allowed, so the deepest wells have larger probability of being considered.



1 Two-dimensional Thompson atomic model

We wanna simulate a system consisting of N Coulomb charges in a two-dimensional harmonic trap where the potential energy is given by:

$$E_{pot} = \sum_{i=1}^{N} \frac{1}{2} m\omega^2 r_i^2 + \sum_{i<j}^{N} \frac{q^2}{|\mathbf{r}_i - \mathbf{r}_j|} \tag{1}$$

Using some convention in units and dimensionless variables. We can write the potential energy as:

$$\tilde{E}_{pot} = \sum_{i=1}^{N} \tilde{r}_i^2 + \sum_{i<j}^{N} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} \tag{2}$$

In two dimensions, it becomes

$$\tilde{E}_{pot} = \sum_{i=1}^{N} (x_i^2 + y_i^2) + \sum_{i<j}^{N} \frac{1}{\sqrt{(x_j - x_i)^2 + (y_j - y_i)^2}} \tag{3}$$

Theoretically, for N particles, the total energy can be approxximated as:

$$\tilde{E} = \left(N^{2/3} - 1\right) \cdot N2^{1/3} \tag{4}$$

This formulation was implemented in Python with the following code

```python
def potential(N, R):
    E = 0
    for i in range(N):
        E += (R[i,0]**2 + R[i,1]**2)
        for j in range(i+1,N):
            E += 1/np.sqrt((R[i,0]-R[j,0])**2 + (R[i,1]-R[j,1])**2)
    return E
```

It has been tested with some fixed configuration, eg $N = 2, r = 0.5 \rightarrow E_{pot} = 1.5$.
We wanna use the classical Monte Carlo method and the annealing method to find the minimal energy configuration.

2 Annealing method

The metropolis algorithm can be implemented by calculating

$$\exp\left\{-\frac{E(\mathbf{R}') - E(\mathbf{R})}{T}\right\} \tag{5}$$

where T is an artificial temperature.

This formulation was implemented in Python with an simple routine

```python
def MaxBoltz(dE, T):
    return math.exp(-(dE)/T)
```

3 Metropolis algorithm

Now we describe briefly the steps of the Metropolis algorithm; starting from a random configuration of N charges.

1. Select a charges
2. Do a random displacement
3. Decide if it has to be accepted or not

```python
def MoveOneParticle(N,R,T,dt):
    R_new = R.copy()
    # Random choice of one charge to move
    i = np.random.randint(N)
    # Do a random displacement
    R_new[i] += np.random.rand(2) * dt - dt/2
    # Potential energy difference calculation
    dE = potential(N, R_new) - potential(N, R)
    # Acceptance or rejection of the new position based on the metropolis algorithm
    if dE < 0:
      return R_new
    else:
      p_acc = MaxBoltz(dE, T)
      if np.random.rand() < p_acc:
        return R_new
      else:
        return R
```

```python
def MoveAllParticles(N,R,T,dt):
    R_new = R.copy()
    # Do a random displacement
    for i in range(N):
      R_new[i] += np.random.rand(2) * dt - dt/2
    # Potential energy difference calculation
    dE = potential(N, R_new) - potential(N, R)
    # Acceptance or rejection of the new position based on the metropolis algorithm
    if dE < 0:
      return R_new
    else:
      p_acc = MaxBoltz(dE, T)
      if np.random.rand() < p_acc:
        return R_new
      else:
        return R
```

```python
while T > Tf:
  pbar.update()
  for _ in range(1000):
    R = MoveOneParticle(N, R, T, dt)
  for _ in range(100):
    R = MoveAllParticles(N, R, T, dt)
  T *= cooling_rate
  Temp[i] = T
  E[i] = potential(N, R)
  i += 1
```

4 Results - *N=5*

We simulate a system of $N = 5$ charges with the following parameters:

- Start temperature: $T_0 = 10$
- Final temperature: $T_f = 0.01$
- Temperature step: $\delta_T = 0.995$
- Displacement amplitude: $\Delta t = 0.5$
- Monte Carlo iterations for each temperature step: $N_{iter} = 10000$

For $N = 5$ particles, the total energy should be $\tilde{E} \approx 2.33845 \cdot N = 11.6922$ and the particles should be in one single shell structure.

In the Figure 1 we have plotted the energy dependence during iterations and the temperature.

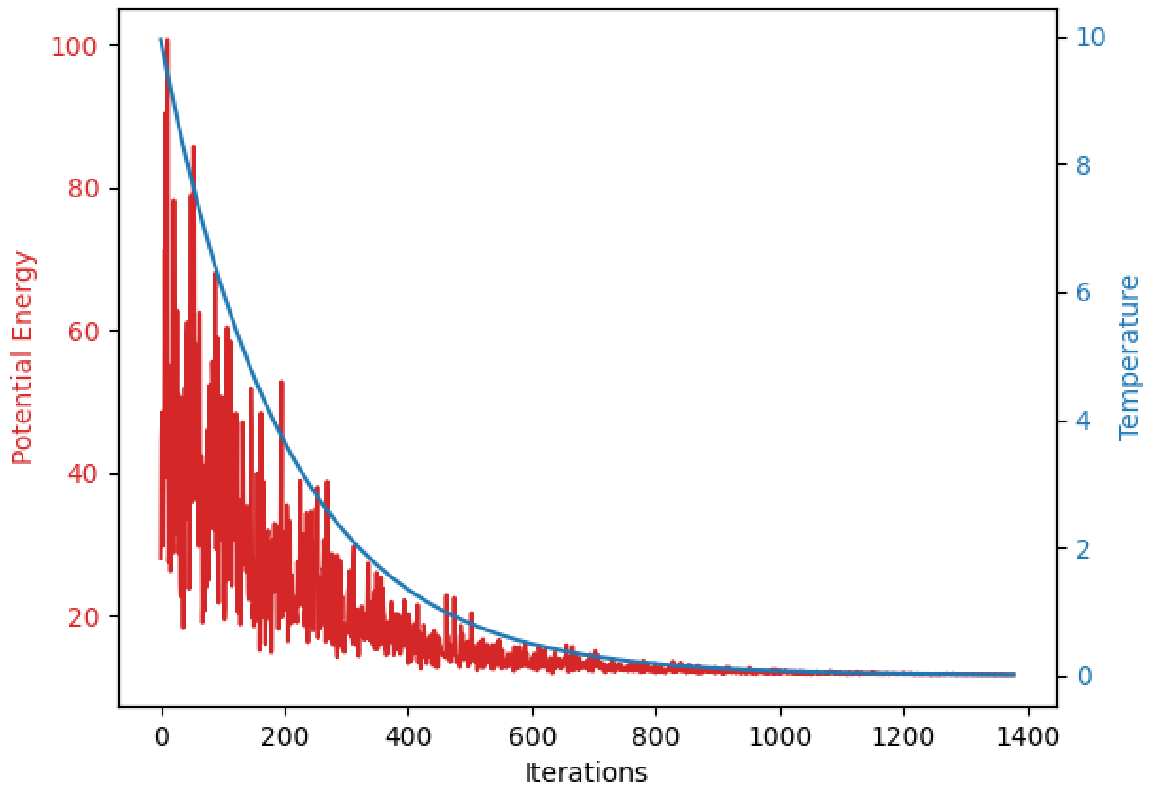


Figure 1: Potential Energy and Temperature over Iterations

We can easily appreciate that the value of the potential energy tends rapidly toward the optimal value.

In the Figure 2 we have plotted the snapshot of the optimal configuration for $N = 5$ charges.

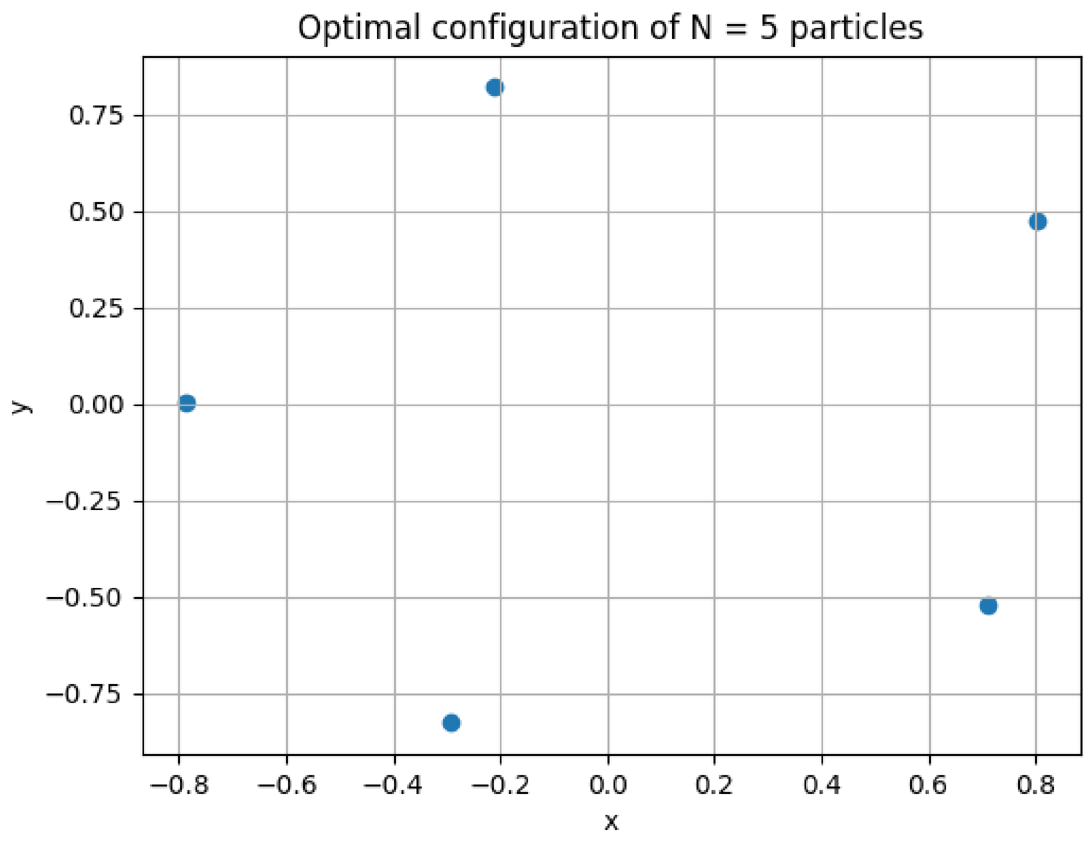


Figure 2

As we can see the charges lies on a single shells centred in $(0, 0)$, forming a pretty regular pentagon.

We have computed the average value of the last 100 iteration, the value of the potential energy at the optimal configuration is: $\tilde{E}_{opt} = 11.7453$. The absolute minimum energy value found in an iteration is $E_{min} = 11.7046$.

5 Results - *N=20*

We simulate a system of $N = 20$ charges with the following parameters:

- Start temperature: $T_0 = 10$
- Final temperature: $T_f = 0.01$
- Temperature step: $\delta_T = 0.995$
- Displacement amplitude: $\Delta t = 0.5$
- Monte Carlo iterations for each temperature step: $N_{iter} = 10000$

For $N = 20$ particles, the total energy should be $\tilde{E} \approx 7.94961 \cdot N = 158.922$ and the particles should be in tree shell structure, in particular $N_1 = 1, N_2 = 7, N_3 = 12$.

In the Figure 3 we have plotted the energy dependence during iterations and the temperature.

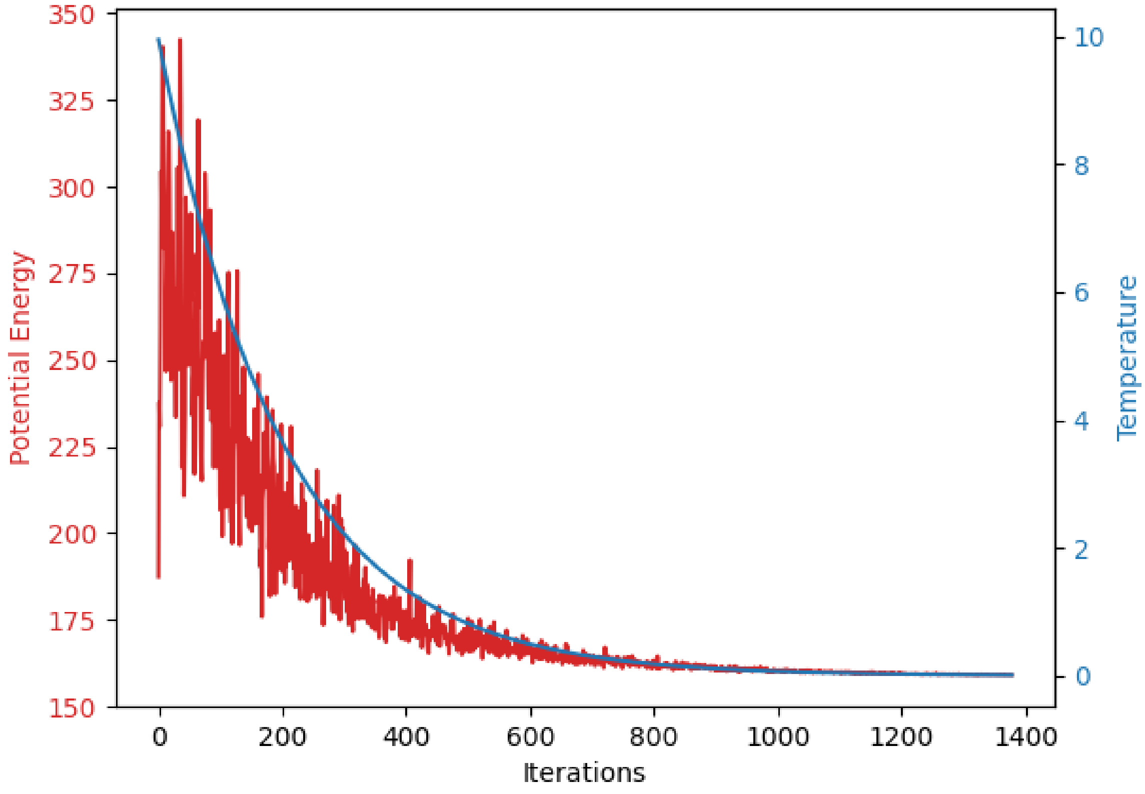


Figure 3: Potential Energy and Temperature over Iterations

Again, we appreciate that the value of the potential energy tends rapidly toward the optimal value.

In the Figure 4 we have plotted the snapshot of the optimal configuration for $N = 20$ charges.

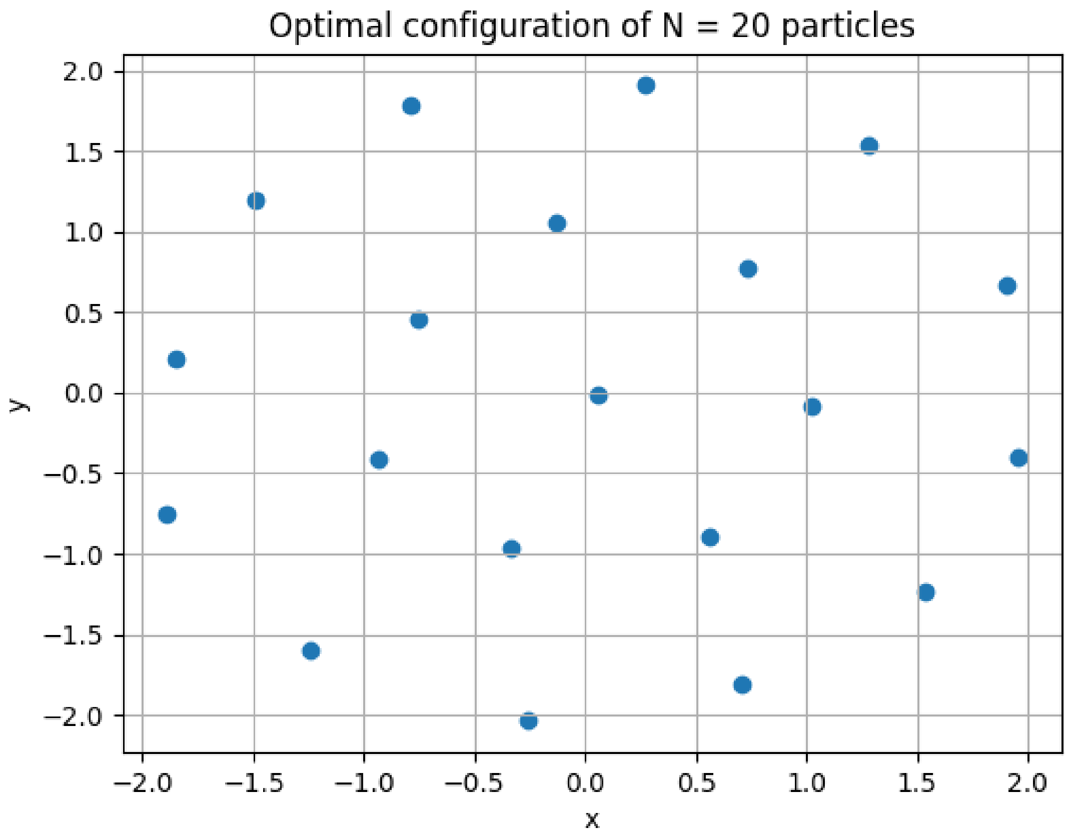


Figure 4

As we can see, the charges are arranged in a double-shell configuration centred at $(0, 0)$. As expected, at the centre, there is only one charge, while the first shell contains 7 charges, and the second shell contains 12 charges. Together, they form a more complex yet still regular structure.

Moreover, we have computed the average value of the last 100 iterations. The value of the potential energy at the optimal configuration is $\tilde{E}_{\text{opt}} = 159.2435$. Additionally, the absolute minimum energy value found in any single iteration is $E_{\text{min}} = 159.1289$. These values provide insights into the stability and convergence of the system.

6 Results - *N=26*

We simulate a system of $N = 26$ charges with the following parameters:

- Start temperature: $T_0 = 10$
- Final temperature: $T_f = 0.01$
- Temperature step: $\delta_T = 0.995$
- Displacement amplitude: $\Delta t = 0.5$
- Monte Carlo iterations for each temperature step: $N_{iter} = 10000$

For $N = 26$ particles, the total energy should be $\tilde{E} \approx 9.76273 \cdot N = 253.831$ and the particles should be in tree shell structure, in particular $N_1 = 3, N_2 = 9, N_3 = 14$.

In the Figure 5 we have plotted the energy dependence during iterations and the temperature.

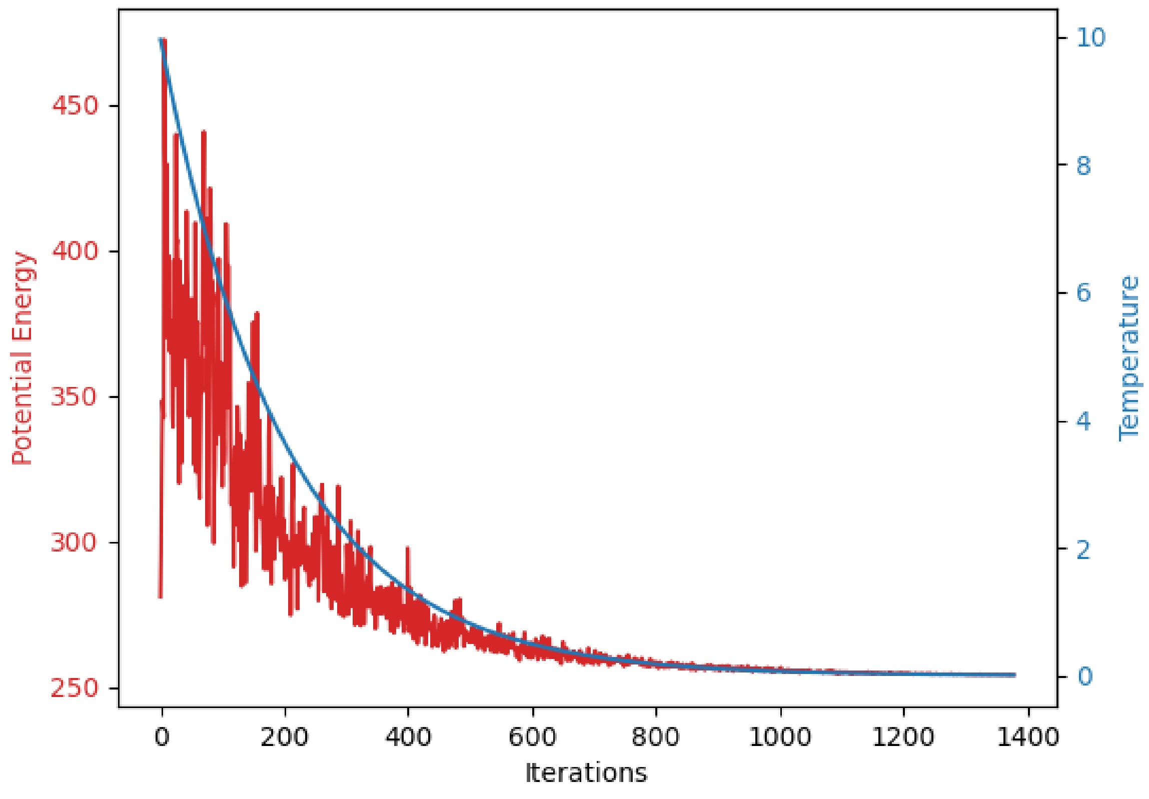


Figure 5: Potential Energy and Temperature over Iterations

Again, we appreciate that the value of the potential energy tends rapidly toward the optimal value.

In the Figure 6 we have plotted the snapshot of the optimal configuration for $N = 26$ charges.

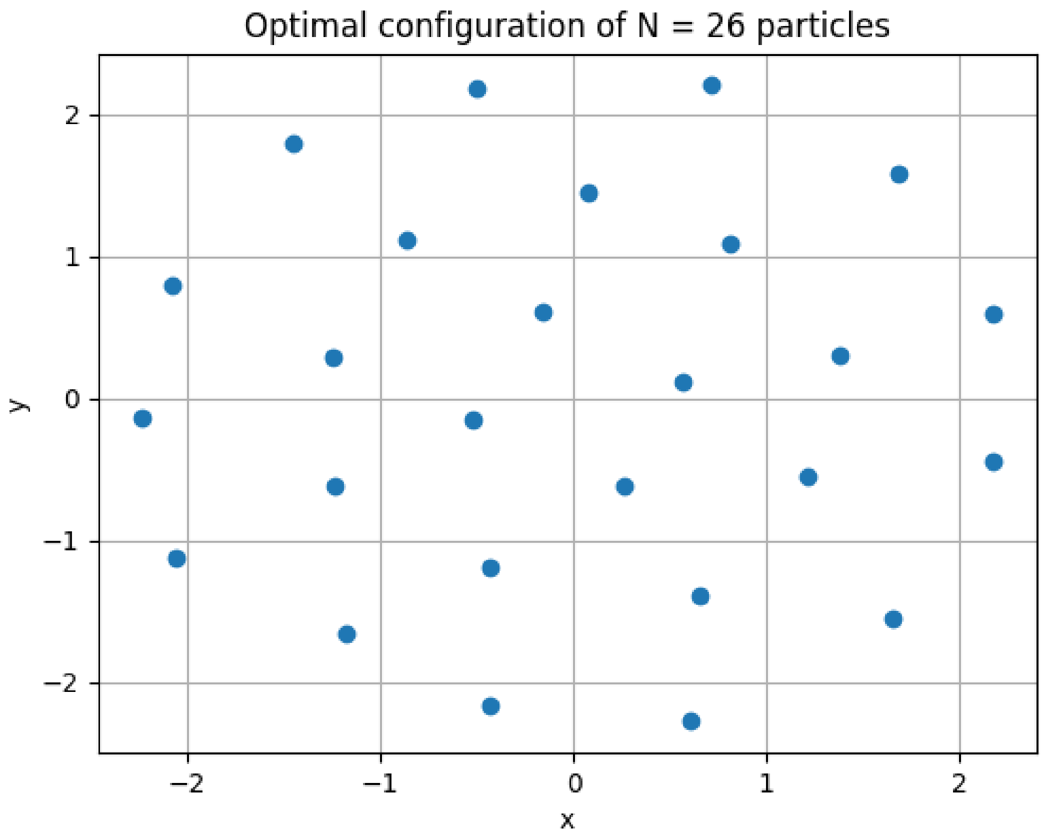


Figure 6

We can appreciate that the charges are arranged in a double-shell configuration centred at $(0, 0)$. Together, they form a more complex yet still regular structure.

We have computed the average value of the last 100 iteration, the value of the potential energy at the optimal configuration is: $\tilde{E}_{opt} = 254.1912$. The absolute minimum energy value found in an iteration is $E_{min} = 254.0370$.

7 Conclusions

Finally we compare the obtained results with the one provided in the literature.

N	Simulations E/N	Literature E/N
5	2.3491	2.33845
20	7.9622	7.94961
26	9.7766	9.76273

Table 1: Comparing obtained results with reference data