In [2]:
```python
import numpy as np
import time
import matplotlib.pyplot as plt
from mpl_toolkits import mplot3d
```

AM 307 HW3

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Question 1: Gradient based against evolution strategy

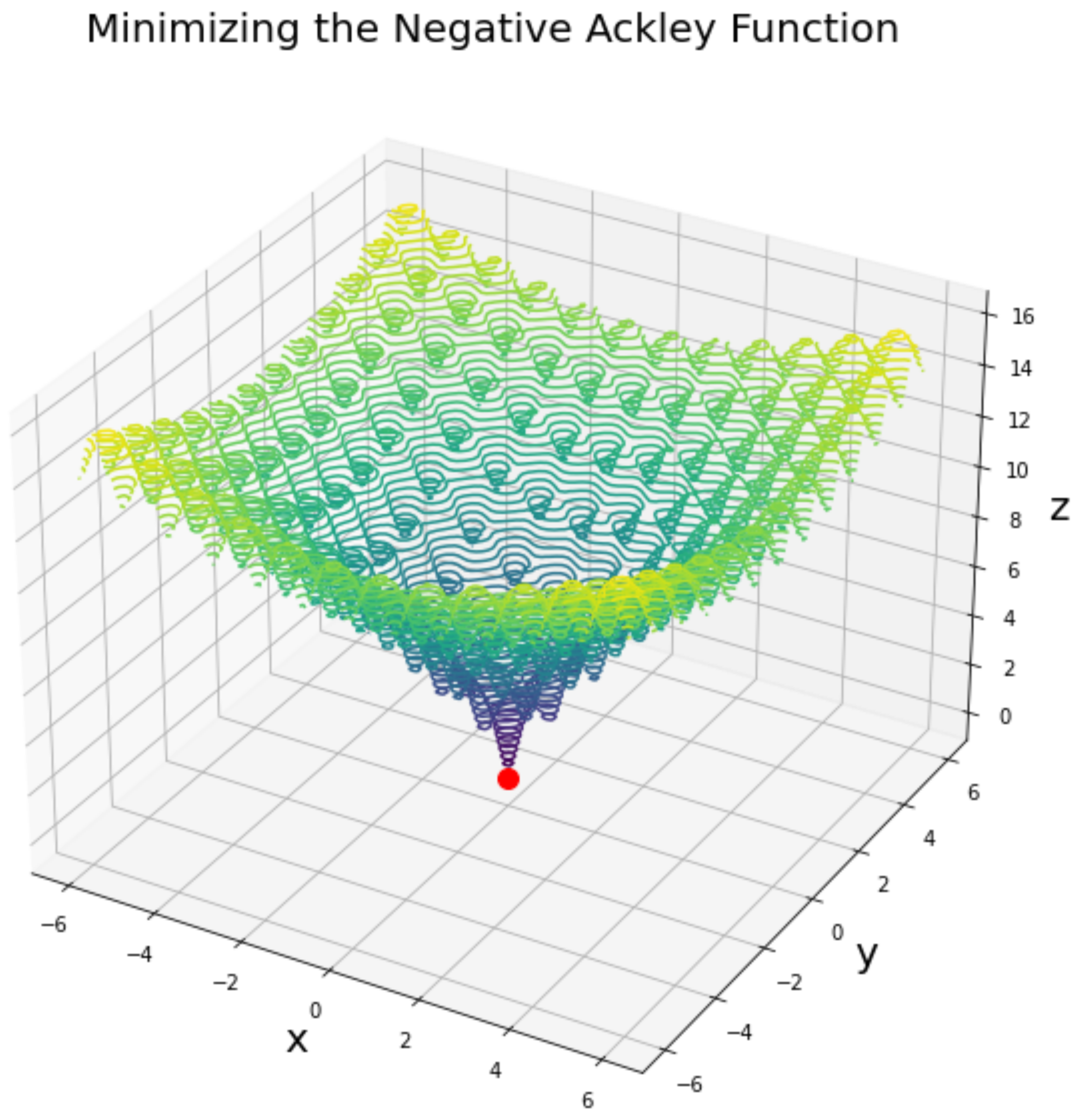
We consider the negative Ackley function in two dimensions :

$$f(x,y) = -20\exp(-0.2\sqrt{0.5(x^2 + y^2)}) - \exp(0.5*(\cos(2\pi x) + \cos(2\pi y))) + 20 + e$$ where $x, y \in \mathbb{R}$, and e is the Euler number.

We know that the korali CMA-ES implemented in the given package maximises functions. Hence, in order to minimise the function f here-above, we must aim to maximise $-f$.

In [205…
```python
def negative_ackley(X,Y):
    a = 20.
    b = 0.2
    c = 2.*np.pi
    x = [X, Y]
    dim = len(x)

    sum1 = 0.
    sum2 = 0.
    for i in range(dim):
        sum1 += x[i]*x[i]
        sum2 += np.cos(c*x[i])

    sum1 /= dim
    sum2 /= dim
    r1 = a*np.exp(-b*np.sqrt(sum1))
    r2 = np.exp(sum2)

    return - (r1 + r2 - a - np.exp(1))
```

In [283…
```python
x = np.linspace(-6, 6, 100)
y = np.linspace(-6, 6, 100)


X, Y = np.meshgrid(x, y)
Z = negative_ackley(X, Y)

fig = plt.figure(figsize=(10,10))
ax = plt.axes(projection='3d')
ax.scatter([0], [negative_ackley(0,0)], c ='r', s = 100)

ax.contour3D(X, Y, Z, 50, cmap='viridis')
ax.set_xlabel('x', fontsize = 20)
ax.set_ylabel('y', fontsize = 20)
ax.set_zlabel('z', fontsize = 20)
ax.set_title('Minimizing the Negative Ackley Function', fontsize = 20)
plt.show()
```

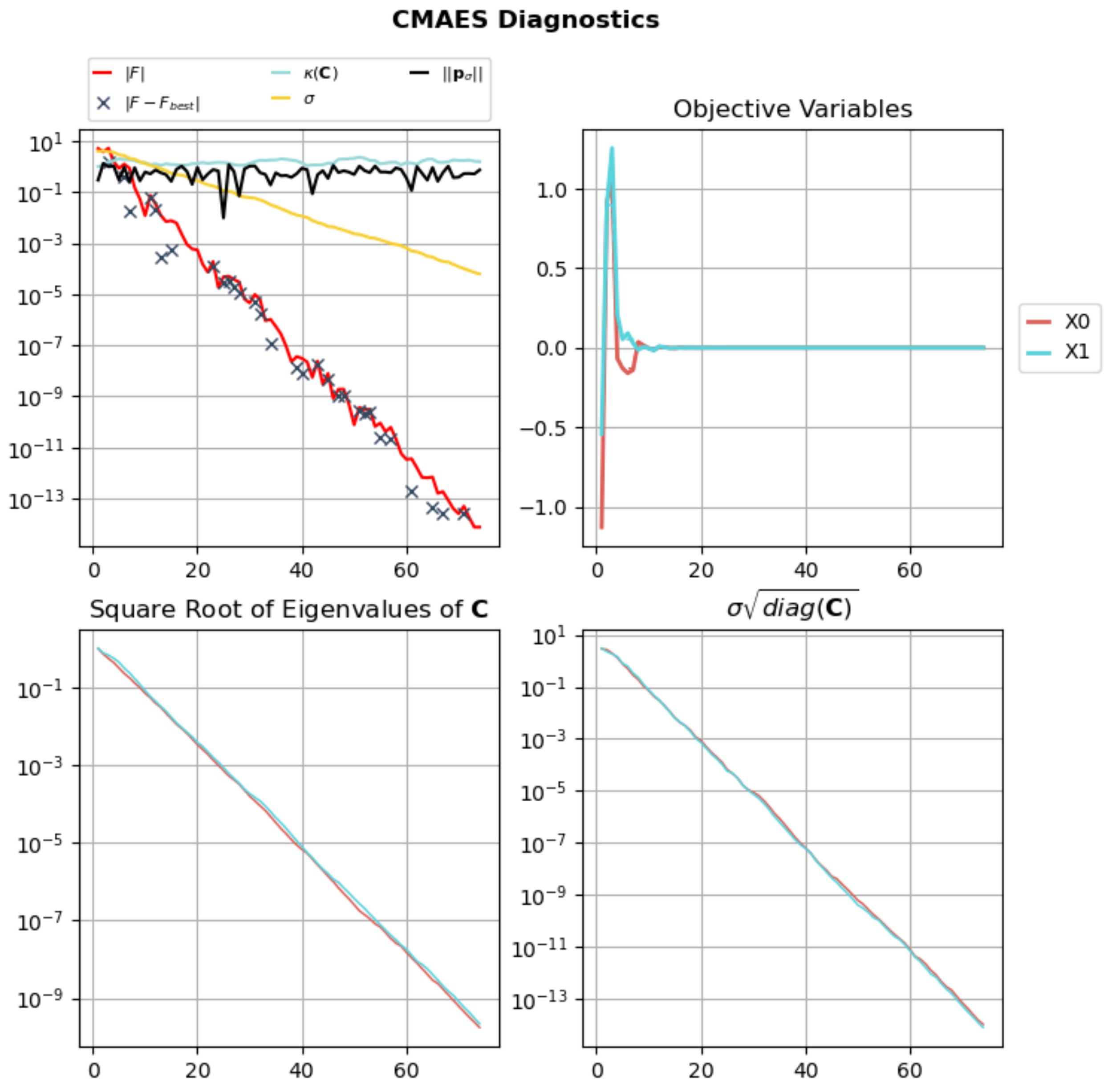


In [192…
```
negative_ackley(0,0)
```
Out[192]:
```
4.440892098500626e-16
```

The minimum seems to be located at $(0,0)$. We have that $f(0,0) = 0$.

a) Evolution Strategy : CMA-ES

Using CMA-ES, we find a minimum of $-7.549517\times 10^{-15} \approx 0$ located at $(X_0,Y_0) = \left (6.244\times 10^{-16}, -2.273\times 10 ^{-15}\right) \approx (0,0) $. This confirms our observation here-above. The convergence plot of our algorithm can be found here-under.



b) Gradient Based Method

Let us compute the analytical expression of the negative ackley function's gradient.

We have that : $$f(x,y) = -20\exp(-0.2\sqrt{0.5(x^2 + y^2)}) - \exp(0.5*(\cos(2\pi x) + \cos(2\pi y))) + 20 + e$$ where $x, y \in \mathbb{R}$, and e is the Euler number.

Then,

$$\frac{\partial f}{\partial x}(x,y) = \frac{2x}{\sqrt{0.5(x^2 + y^2)}}\exp(-0.2\sqrt{0.5(x^2 + y^2)}) + \pi \sin(2 \pi x)\exp(0.5*(\cos(2\pi x) + \cos(2\pi y))) $$
\ $$\frac{\partial f}{\partial y}(x,y) = \frac{2y}{\sqrt{0.5(x^2 + y^2)}}\exp(-0.2\sqrt{0.5(x^2 + y^2)}) + \pi \sin(2 \pi y)\exp(0.5*(\cos(2\pi x) + \cos(2\pi y)))$$

and we have that :

$$\nabla f(x, y) = \left [\frac{\partial f}{\partial x}(x,y),\frac{\partial f}{\partial y}(x,y) \right]^T$$

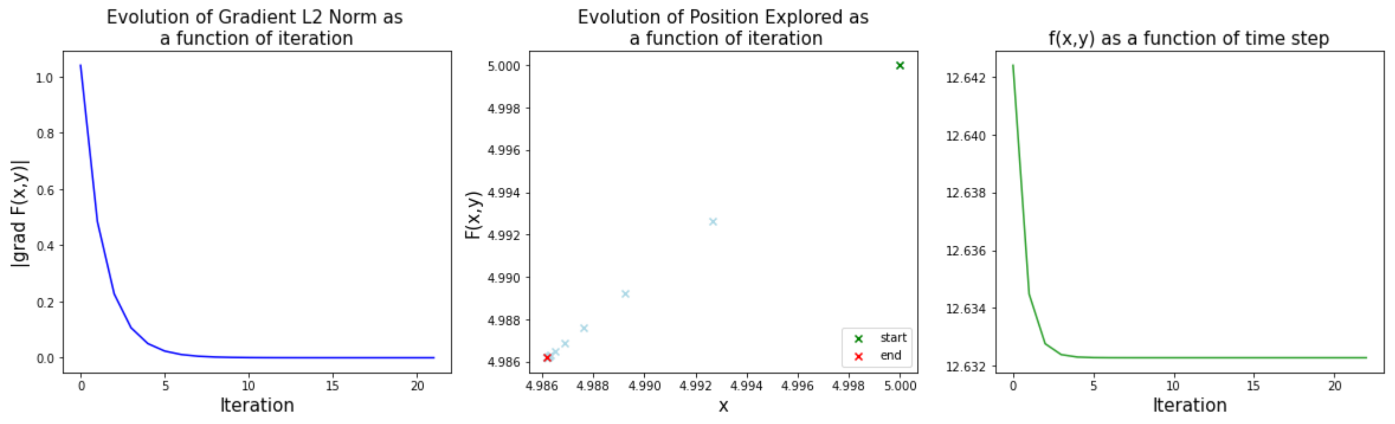
```
In [347…
def grad(X):
    x = X[0]
    y = X[1]
    grad_x = 2*x* np.exp(-0.2*np.sqrt(0.5*(x**2 + y**2)))/(np.sqrt(0.5*(x**2 + y**2))) +
    grad_y = 2*y* np.exp(-0.2*np.sqrt(0.5*(x**2 + y**2)))/(np.sqrt(0.5*(x**2 + y**2))) +
    return np.array([grad_x, grad_y])

old = 100
new = 0
eps = 1e-32
X = np.array([5,5])
x = X[0]
y = X[1]
t = 0
max_iter  = 300
alpha = 0.01
grads = []
positions = [[x, y]]

while abs(old - new) > eps and t <max_iter :
    old = negative_ackley(x, y)
    gradient = grad(X)
    grads.append(gradient)
    X = X - alpha*gradient
    x = X[0]
    y = X[1]
    positions.append([x,y])
    t += 1
    new = negative_ackley(x, y)


x_pos = [i[0] for i in positions]
y_pos = [i[1] for i in positions]

evals = [negative_ackley(i[0], i[1]) for i in positions]

print('Iterations: ', t)
print('Final position: ', X)
print('Minimum value found: ', negative_ackley(X[0], X[1]))
```

```
Iterations:  22
Final position:  [4.98618046 4.98618046]
Minimum value found:  12.632268991516
```

```
In [292…
fig, axs = plt.subplots(1, 3)
fig.set_figheight(5)
fig.set_figwidth(20)
norms_grad = [np.linalg.norm(i) for i in grads]

axs[0].plot(range(t), norms_grad, label = 'norm of gradient',c = 'b')
axs[0].set_title('Evolution of Gradient L2 Norm as \na function of iteration', fontsize
axs[0].set_xlabel('Iteration', fontsize = 15)
axs[0].set_ylabel('|grad F(x,y)|', fontsize = 15)

axs[1].scatter(x_pos, y_pos, c = 'lightblue', marker = 'x')
axs[1].scatter(x_pos[0], y_pos[0], c = 'g', marker = 'x', label = 'start')
axs[1].scatter(x_pos[-1], y_pos[-1], c = 'r', marker = 'x', label = 'end')
axs[1].set_title('Evolution of Position Explored as\n a function of iteration', fontsize
axs[1].set_xlabel('x', fontsize = 15)
axs[1].set_ylabel('y', fontsize = 15)
axs[1].legend(loc = 'lower right')

axs[2].plot(range(t + 1), evals, 'tab:green')
axs[2].set_title('f(x,y) as a function of time step', fontsize = 15)
axs[2].set_xlabel('Iteration', fontsize = 15)
axs[1].set_ylabel('F(x,y)', fontsize = 15)
```

```
print('Convergence Plots for Our gradient Based Method')

plt.show()
```

```
Convergence Plots for Our gradient Based Method
```

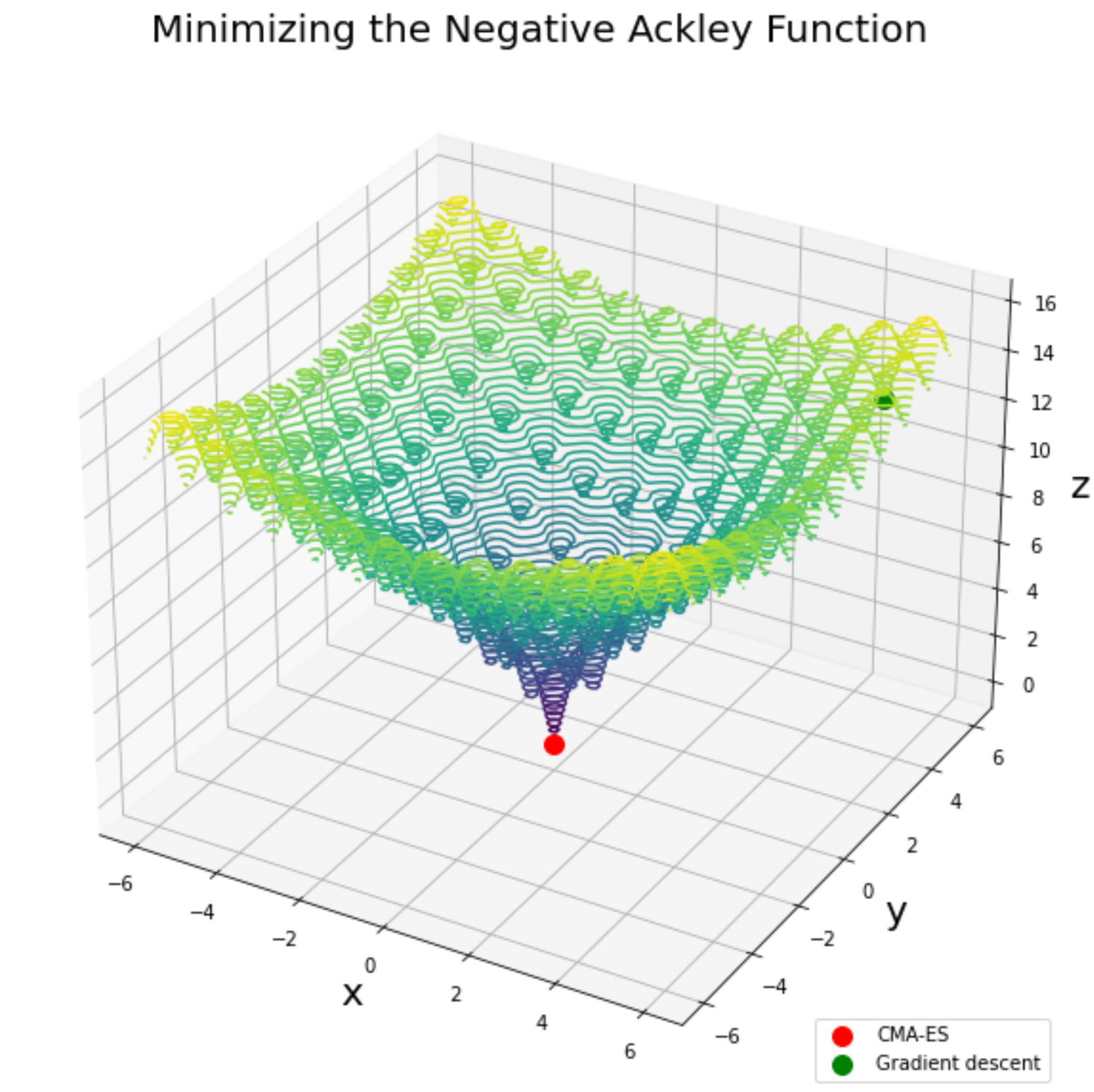


In [302…

```
x = np.linspace(-6, 6, 100)
y = np.linspace(-6, 6, 100)



X, Y = np.meshgrid(x, y)
Z = negative_ackley(X, Y)

fig = plt.figure(figsize=(10,10))
ax = plt.axes(projection='3d')
ax.scatter([0], [negative_ackley(0,0)], c ='r', label = 'CMA-ES', s = 100)
ax.scatter([x_pos[-1]], [y_pos[-1]], [negative_ackley(x_pos[-1], y_pos[-1])], c ='g', la


ax.contour3D(X, Y, Z, 50, cmap='viridis')
ax.set_xlabel('x', fontsize = 20)
ax.set_ylabel('y', fontsize = 20)
ax.set_zlabel('z', fontsize = 20)
ax.set_title('Minimizing the Negative Ackley Function', fontsize = 20)
ax.legend(loc = 'lower right')
plt.show()
```

```python
#!/usr/bin/env python3
import korali
import math
import numpy as np

def negative_ackley(p):
    ''' this function returns -f where f is the function given in the homework sheet
        korali will maximise -f i.e minimise f.
    '''
    x = p["Parameters"]
    a = 20.
    b = 0.2
    c = 2.*np.pi
    dim = len(x)

    sum1 = 0.
    sum2 = 0.
    for i in range(dim):
        sum1 += x[i]*x[i]
        sum2 += np.cos(c*x[i])

    sum1 /= dim
    sum2 /= dim
    r1 = a*np.exp(-b*np.sqrt(sum1))
    r2 = np.exp(sum2)

    p["F(x)"] = r1 + r2 - a - np.exp(1)

    grad = [0.]*dim
    for i in range(dim):
      grad[i] = r1*-1*b*0.5/np.sqrt(sum1)*1.0/dim*2.0*x[i]
      grad[i] -= r2*1.0/dim*np.sin(c*x[i])*c

    p["Gradient"] = grad

k = korali.Engine()
e = korali.Experiment()

# Configuring Problem
e["Random Seed"] = 0xC0FEE
e["Problem"]["Objective Function"] = negative_ackley
e["Problem"]["Type"] = "Optimization"

dim = 2

# Defining the problem's variables.
for i in range(dim):
    e["Variables"][i]["Name"] = "X" + str(i)
    e["Variables"][i]["Initial Value"] = 5
    e["Variables"][i]["Lower Bound"] = -32.768
    e["Variables"][i]["Upper Bound"] = 32.768
    e["Variables"][i]["Initial Standard Deviation"] = 5
    e["Variables"][i]["Initial Mean"] = 5


# Configuring CMA-ES parameters
e["Solver"]["Type"] = "Optimizer/CMAES"
e["Solver"]["Population Size"] = 32
e["Solver"]["Mu Value"] = 8

e["Solver"]["Termination Criteria"]["Min Value Difference Threshold"] = 1e-32
e["Solver"]["Termination Criteria"]["Max Generations"] = 200

# Configuring results path
e["File Output"]["Enabled"] = True
e["File Output"]["Path"] = '_korali_result_cmaes'
e["File Output"]["Frequency"] = 1
```

```
# Running Korali
k.run(e)
```



We can see that our gradient descent method falls in the trap of a local minima whereas CMA-ES manage sto find the global minimum even though the initial positions are the same : $(5,5)$. We could improve our gradient based method by perhapse modifying our hyperparameter α as $\alpha(x, y, t)$ and make it vary as a function of the position and tiime step to ensure that our step size changes based on the functional context.

Question 2: Corridor design for pedestrian traffic

The file ex2a.cpp runs a simulation of pedestrian traffic for given initial conditions.

The file ex2b.cpp consists in the application of a differential algorithm to find the obstacle positions that maximise pedestrian horizontal displacement.

a)

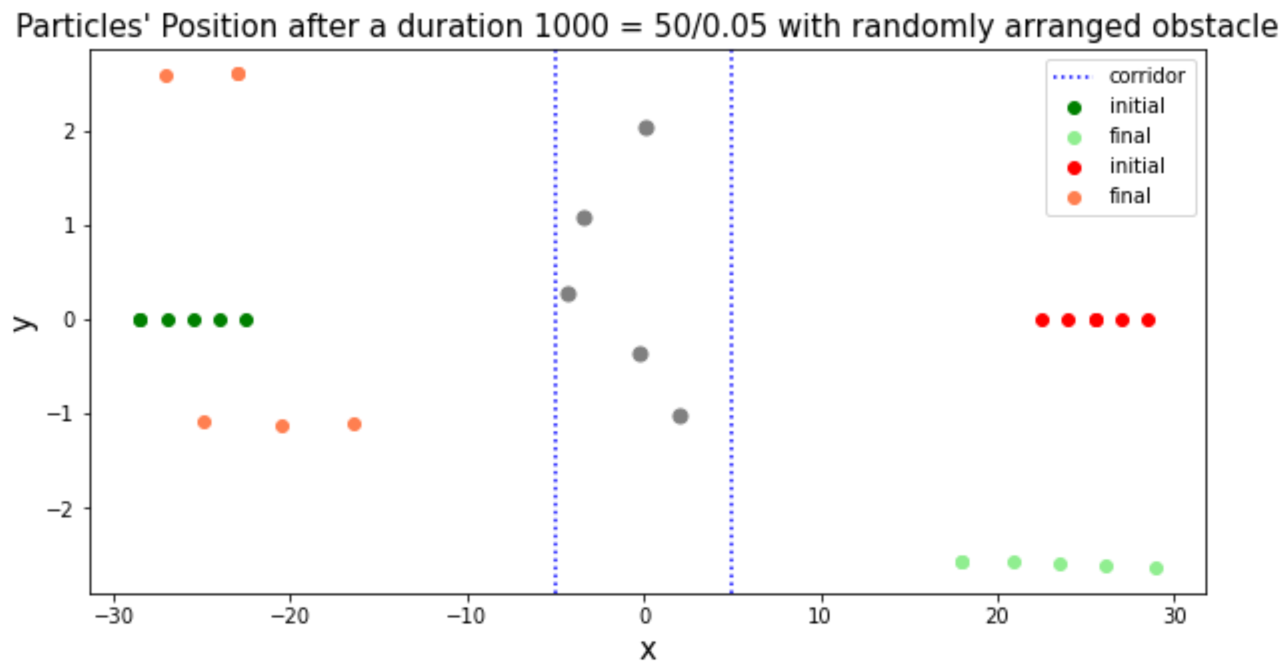
Here, we run the simulation with a randomly generated set of obstacle positions.

```
In [326…
def average_x_displacement(X_2, X_1):
    sum = 0
    for i in range(10):
        sum += abs(X_2[i][0] - X_1[i])
    return sum/10

def plot_corridor(X_init, X_fin, obstacles, title_name = "Particles' Position after a du

    fig = plt.figure(figsize=(10,5))

    for i in range(10):
        if i < 5:
            plt.scatter(X_init[i],Y_init[i], c = 'g' )
            plt.scatter(obstacles[i][0],obstacles[i][1], c = 'grey' ,s = 50)
            plt.scatter(X_fin[i][0],X_fin[i][1], c = 'lightgreen' )
        else:
            plt.scatter(X_fin[i][0],X_fin[i][1], c = 'coral')
            plt.scatter(X_init[i],Y_init[i], c = 'r')
    plt.axvline(x = -5, color = 'b', linestyle =":")
    plt.axvline(x = 5, color = 'b', linestyle =":", label = 'corridor')
    plt.scatter(X_init[0],Y_init[0], c = 'g', label = 'initial')
    plt.scatter(X_fin[0][0],X_fin[0][1], c = 'lightgreen', label = 'final')
    plt.scatter(X_init[7],Y_init[7], c = 'r', label = 'initial')
    plt.scatter(X_fin[7][0],X_fin[7][1], c = 'coral', label = 'final')
    plt.xlabel('x', fontsize = 15)
    plt.ylabel('y', fontsize = 15)
    plt.title(title_name, fontsize = 15)
    plt.legend(loc = 'best')
    plt.show()
```

In [328…

```
X_init = [-28.5, -27.0, -25.5, -24.0, -22.5, 22.5, 24.0, 25.5, 27.0, 28.5]
Y_init = [0]*len(X_init)

### the following were generated randomly

obstacles = np.array( [[-3.39921,1.08641],
[0.0510252,2.04437],
[-0.29937,-0.361777],
[-4.27294,0.268635],
[2.00433,-1.01766]])


### these final points have been found by running our model in ex2a.cpp

X_fin = np.array(  [[18.0225,-2.56035],
[20.8957,-2.56163],
[23.5264,-2.57656],
[26.1259,-2.6085],
[28.9008,-2.63531],
[-27.0298,2.58878],
[-24.9074,-1.08022],
[-23.0161,2.59947],
[-20.5377,-1.12527],
[-16.4598,-1.1081]])
displacement =  average_x_displacement(X_fin, X_init)
print('Average horizontal displacement is : ',displacement)
plot_corridor(X_init, X_fin, obstacles, "Particles' Position after a duration 1000 = 50/
```

```
Average horizontal displacement is :  48.44221
```



b)

We want to find the positions of the 5 obstacles that maximise the average displacement of the particles in the x direction. We want to maxmise the function f as : $$f(\underline{x}(T), \underline{x}_0) = \frac{1}{10}\sum_{i}^{10}\lvert x_i(T) - x_i(0)\rvert$$ where T is final time. Let us now find the best obstacle positions to maximise the horizontal displacement over T = $50 /\delta t = 1000$ where $\delta t = 0.05$.

Using the differential evolution algorithm, with $NP = 8$, we obtain the following best positions for the obstacles.

In [348…

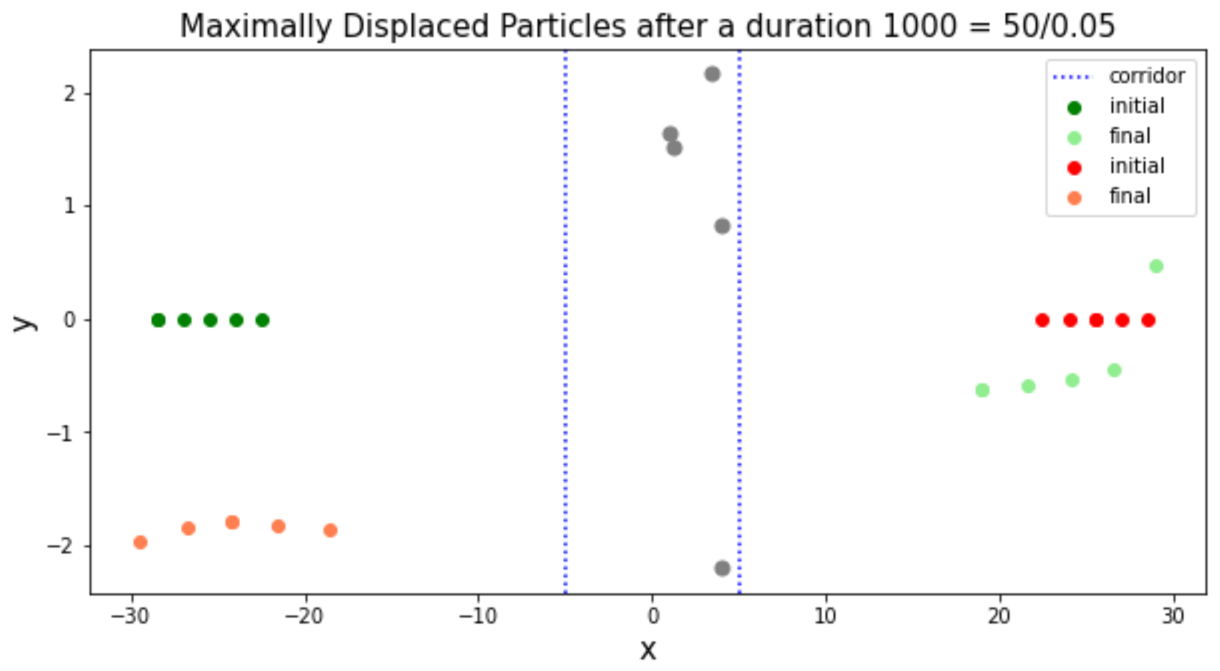
```
best_obstacles = np.array( [[3.40922,2.16217],
[3.99883,0.829755],
[3.98005,-2.20237],
[1.0691,1.63956],
[1.23513,1.51946]] )


X_fin_2 = np.array( [[18.9918,-0.617195],
[21.6715,-0.592555],
[24.1162,-0.536414],
[26.5343,-0.447381],
[28.9612,0.465551],
[-29.4666,-1.97164],
[-26.7702,-1.83248],
[-24.2249,-1.78777],
[-21.6046,-1.82696],
[-18.6108,-1.86264]])


max_displacement = average_x_displacement(X_fin_2, X_init)
print('Maximal average horizontal displacement is : ', max_displacement)
plot_corridor(X_init, X_fin_2, best_obstacles, title_name = "Maximally Displaced Particl
```

```
Maximal average horizontal displacement is :  49.595209999999994
```

```
#include <iostream>
#include <cstdlib>
#include <cmath>
#include <vector>
#include <random>
#include <fstream>
#include <sstream>
#include <string>
#include <algorithm>
#include <format>
#include <random>
using namespace std;

vector <double> compute_F_i(double tau,int N, double A, double B, double C, double D, int
i,vector <double> v_x0, vector <double> v_y0, vector <double> x, vector <double> y, vector
<double> v_x, vector <double> v_y,  vector <double> o_x, vector <double> o_y);


int main()
{
    //hyperparameters

    int N = 10;
    double tau = 0.2;
    double A = 20.;
    double B = 0.5;
    double C = 10.;
    double D = 0.6;
    int O = 5;
    double delta_t = 0.05;
    int max_time = 1000;
    double high_y = 3.;
    double low_y = -3;
    mt19937 gen(20);

   // initialise positions
    vector <double> x {-28.5, -27.0, -25.5, -24.0, -22.5, 22.5, 24.0, 25.5, 27.0, 28.5};
    vector <double>  y {0., 0., 0., 0., 0., 0., 0., 0., 0., 0.};

    vector <double>  x0  {-28.5, -27.0, -25.5, -24.0, -22.5, 22.5, 24.0, 25.5, 27.0, 28.5};
    vector <double>  y0 {0., 0., 0., 0., 0., 0., 0., 0., 0., 0.};

    // initialise velocities
    vector <double> v_x0 {1., 1., 1., 1., 1., -1, -1, -1, -1, -1};
    vector <double> v_y0 {0., 0., 0., 0., 0., 0., 0., 0., 0., 0.};

    vector <double> v_x {1., 1., 1., 1., 1., -1, -1, -1, -1, -1};
    vector <double> v_y  {0., 0., 0., 0., 0., 0., 0., 0., 0., 0.};

    // create obstacles

    // if you already know the positions of your obstacles
    // vector <double> o_x {-3.39921,0.0510252,-0.29937,-4.27294,2.00433};

    // vector <double> o_y {1.08641,2.04437,-0.361777,0.268635,-1.01766};


    // generate random obstacles
    vector <double> o_x (5);
    vector <double> o_y (5);

    uniform_real_distribution < double> distrib_x(-5 + D,5 - D);
    uniform_real_distribution < double> distrib_y(-3 + D,3 - D);

    for (int i = 0; i < 5 ; i++){
            o_x[i] = distrib_x(gen);
  }
```

```cpp
    for (int i = 0; i < 5 ; i++){
            o_y[i] = distrib_y(gen);
  }

    cout << "Obtsacles : [";
    for(int i = 0;i < 5; i++){
        if(i == 4){
            cout << "["<<o_x[i] << "," << o_y[i]<< "]";
        }
        else{
            cout << "["<<o_x[i] << "," << o_y[i]<< "],\n";
        }
    }
    cout << "]\n\n";

    // initialise force

    vector <double> F_i (2);

    for (int time = 0; time < max_time ; time++){
        for(int i = 0;  i < N; i++){
            F_i   = compute_F_i(tau, N, A, B, C, D, i, v_x0, v_y0, x, y, v_x, v_y, o_x, o_y);
            // cout << "F_i_y is :" << F_i[1]<< "\n";
            double F_i_x = F_i[0];
            double F_i_y = F_i[1];
            x[i] += v_x[i]*delta_t;
            y[i] += v_y[i]*delta_t;

            v_x[i] += F_i_x*delta_t;
            v_y[i] += F_i_y*delta_t;

            if (y[i]>high_y){
                y[i] = high_y;
                }
            if (y[i]<low_y){
                y[i] = low_y;
            }
        }
    }
    cout << "Final Points:\n [";
    for(int i = 0;i < 10; i++){
        if(i == 9){
            cout << "["<<x[i] << "," << y[i]<< "]";
        }
        else{
            cout << "["<<x[i] << "," << y[i]<< "],\n";
        }
    }
    cout << "]\n";

    return 0;
}

vector <double> compute_F_i(double tau, int N, double A, double B, double C, double D, int
i,vector <double> v_x0, vector <double> v_y0, vector <double> x, vector <double> y, vector
<double> v_x, vector <double> v_y,  vector <double> o_x, vector <double> o_y){

    vector <double> F_i (2);
    double rik = 0;
    double rij = 0;
    double sum_x = (1/tau)*(v_x0[i] - v_x[i]);
    double sum_y = (1/tau)*(v_y0[i] - v_y[i]);
    for (int j = 0; j< N; j++){
        if (i != j){
            rij = sqrt(pow(x[i] - x[j],2) + pow(y[i] - y[j], 2));
            sum_x += A*exp(-rij/B)*(x[i] - x[j])/rij;
            sum_y += A*exp(-rij/B)*(y[i] - y[j])/rij;
        }
    }

    for (int k = 0; k< 5; k++){
        rik = sqrt(pow(x[i] - o_x[k],2) + pow(y[i] - o_y[k], 2));
        sum_x += C*exp(-rik/D)*(x[i] - o_x[k])/rik;
        sum_y += C*exp(-rik/D)*(y[i] - o_y[k])/rik;
    }
    F_i[0] = sum_x;
    F_i[1] = sum_y;
    return F_i;
}
```

```cpp
#include <iostream>
#include <cstdlib>
#include <cmath>
#include <vector>
#include <random>
#include <fstream>
#include <sstream>
#include <string>
#include <algorithm>
#include <format>
#include <random>
using namespace std;

vector <double> compute_F_i(double tau,int N, double A, double B, double C, double D, int
i,vector <double> v_x0, vector <double> v_y0, vector <double> x, vector <double> y, vector
<double> v_x, vector <double> v_y,  vector <double> o_x, vector <double> o_y);
double average_x_displacement(vector <double>x, vector <double>x0);
vector <double> differential_evolution(int NP, double CR, double F, double tau, int N, int
max_time,
                                    double A, double B, double C, double D, vector <double>
v_x0,
                                    vector <double> v_y0, vector <double> x, vector <double>
y, vector <double> x0 ,vector <double> v_x,
                                    vector <double> v_y,  vector <double> o_x, vector
<double> o_y,
                                    double delta_t, double high_y, double low_y, mt19937
gen);
double f(vector <double> agent, vector <double> x0,vector <double> x, vector <double> y,
        vector <double> v_x0,vector <double> v_y0, vector <double> v_x, vector <double> v_y,
        int N, int max_time,  double tau,  double A, double B, double C, double D, double
delta_t,
        double high_y, double low_y );
int main()
{
    //hyperparameters

    int N = 10;
    int NP = 8;
    double CR = 0.9;
    double F = 0.8;
    double tau = 0.2;
    double A = 20.;
    double B = 0.5;
    double C = 10.;
    double D = 0.6;
    double delta_t = 0.05;
    int max_time = 1000;
    double high_y = 3.;
    double low_y = -3;
    mt19937 gen(20);

   // initialise positions
    vector <double> x {-28.5, -27.0, -25.5, -24.0, -22.5, 22.5, 24.0, 25.5, 27.0, 28.5};
    vector <double> y {0., 0., 0., 0., 0., 0., 0., 0., 0., 0.};

    vector <double>  x0  {-28.5, -27.0, -25.5, -24.0, -22.5, 22.5, 24.0, 25.5, 27.0, 28.5};
    vector <double>  y0 {0., 0., 0., 0., 0., 0., 0., 0., 0., 0.};

    // initialise velocities
    vector <double> v_x0 {1., 1., 1., 1., 1., -1, -1, -1, -1, -1};
    vector <double> v_y0 {0., 0., 0., 0., 0., 0., 0., 0., 0., 0.};

    vector <double> v_x {1., 1., 1., 1., 1., -1, -1, -1, -1, -1};
    vector <double> v_y  {0., 0., 0., 0., 0., 0., 0., 0., 0., 0.};

    // create obstacles
    vector <double> o_x (5);
    vector <double> o_y (5);

    uniform_real_distribution < double> distrib_x(-5 + D,5 - D);
    uniform_real_distribution < double> distrib_y(-3 + D,3 - D);

    for (int i = 0; i < 5 ; i++){
            o_x[i] = distrib_x(gen);
  }
    for (int i = 0; i < 5 ; i++){
            o_y[i] = distrib_y(gen);
  }

    vector <double> best_obstacles(10);
    best_obstacles = differential_evolution(NP, CR, F, tau, N, max_time, A, B, C, D, v_x0,
v_y0, x, y,x0, v_x, v_y, o_x, o_y, delta_t, high_y, low_y, gen);

    cout << "\nbest obstacles : [";
    for(int i = 0;i < 5; i++){
        if(i ==4){
            cout << "["<<best_obstacles[i] << "," << best_obstacles[i + 5]<< "]";
        }
        else{
            cout << "["<<best_obstacles[i] << "," << best_obstacles[i + 5]<< "],\n";
        }
    }
    cout << "]\n\n";
    double best_average_displacement = f(best_obstacles, x0,x,y, v_x0,v_y0, v_x, v_y, N,
max_time, tau,A, B, C, D, delta_t, high_y, low_y );
    cout << "maximal average displacement is : " <<best_average_displacement<< "\n\n";

    cout << "obstacle for c++ : \n{";
    for(int i = 0;i < 10; i++){
        if(i <4){
            cout <<best_obstacles[i] << ",";
        }
        if(i == 4){
            cout <<best_obstacles[i] << "}\n{";
        }
        if (i >= 5 and i < 9){
            cout <<best_obstacles[i]<< ",";
        }
        if (i == 9){
            cout <<best_obstacles[i];
        }
    }
    cout << "}\n\n";


    return 0;
}

vector <double> compute_F_i(double tau, int N, double A, double B, double C, double D, int
i,vector <double> v_x0, vector <double> v_y0, vector <double> x, vector <double> y, vector
<double> v_x, vector <double> v_y,  vector <double> o_x, vector <double> o_y){

    vector <double> F_i (2);
    double rik = 0;
    double rij = 0;
    double sum_x = (1/tau)*(v_x0[i] - v_x[i]);
    double sum_y = (1/tau)*(v_y0[i] - v_y[i]);
    for (int j = 0; j< N; j++){
        if (i != j){
            rij = sqrt(pow(x[i] - x[j],2) + pow(y[i] - y[j], 2));
            sum_x += A*exp(-rij/B)*(x[i] - x[j])/rij;
            sum_y += A*exp(-rij/B)*(y[i] - y[j])/rij;
        }
    }
    for (int k = 0; k< 5; k++){
        rik = sqrt(pow(x[i] - o_x[k],2) + pow(y[i] - o_y[k], 2));
        sum_x += C*exp(-rik/D)*(x[i] - o_x[k])/rik;
        sum_y += C*exp(-rik/D)*(y[i] - o_y[k])/rik;
    }
    F_i[0] = sum_x;
    F_i[1] = sum_y;
    return F_i;
}

double average_x_displacement(vector <double>x, vector <double>x0){
    double sum = 0;
    for(int i = 0;i < 10; i++){
        sum += abs(x[i] - x0[i]);
    }
    return sum/10;
}

vector <double> differential_evolution(int NP, double CR, double F, double tau, int N, int
max_time,
                                    double A, double B, double C, double D, vector <double>
v_x0,
                                    vector <double> v_y0, vector <double> x, vector <double>
y, vector <double> x0, vector <double> v_x,
                                    vector <double> v_y,  vector <double> o_x, vector
<double> o_y,
                                    double delta_t, double high_y, double low_y, mt19937 gen)
{
    // intialise agents obstacles

    uniform_real_distribution < double> distrib_x(-5 + D,5 - D);
    uniform_real_distribution < double> distrib_y(-3 + D,3 - D);
    uniform_real_distribution < double> distrib_r(0,1);
    uniform_int_distribution < int> distrib_agent(0,NP);
    uniform_int_distribution < int> distrib_R(0,10);

    double population[N][NP]; //cols, rows
    for (int coord = 0; coord < N; coord++){
        for (int pop = 0; pop < NP; pop++){
            if(coord < 5){
                population[coord][pop] = distrib_x(gen);
            }
            if(coord >=5){
                population[coord][pop] = distrib_y(gen);
            }
        }
    }

    // termination criterion
    int max_iter = 100;
    int t = 0;
    while(t < max_iter){
        for (int i = 0;i < NP; i++){ // for each agent from agent population
            vector <double> current_agent(10);

            for(int j = 0; j < 10; j++){
                current_agent[j] = population[j][i];
            }

            // make 3 agents a,  b, c
            vector <double> a(10);
            vector <double> b(10);
            vector <double> c(10);

            int a_idx = distrib_agent(gen);
            int b_idx = distrib_agent(gen);
            int c_idx = distrib_agent(gen);
            while(a_idx == b_idx or a_idx == c_idx or c_idx == b_idx or a_idx== i or b_idx ==
i or c_idx == i){
                b_idx = distrib_agent(gen);
                c_idx = distrib_agent(gen);
                a_idx = distrib_agent(gen);
            }

            for(int j = 0; j < 10; j++){
                a[j] = population[j][a_idx];
                b[j] = population[j][b_idx];
                c[j] = population[j][c_idx];
            }

            //get random index in [0,10]
            int R = distrib_R(gen);

            //new potential position for agent
            vector <double> y(10);

            for (int j =0; j < 10; j++){
                double r_j = distrib_r(gen);
                if(r_j < CR or j == R){
                    vector <double> b_c(10);
                    for (int k = 0; k < 10 ; k++){
                        b_c[k] = F*(b[k] - c[k]);
                 }

                    y[j] = a[j]+b_c[j];
                    // cout << y[j]<< "\n";
                }
                if (r_j >= CR and j != R){
                    y[j] = current_agent[j];
                }
            }
            double distance_y = f(y, x0,x,y, v_x0,v_y0, v_x, v_y, N,  max_time, tau,A, B, C,
D, delta_t, high_y, low_y );
            double distance_current_agent = f(current_agent, x0,x,y, v_x0,v_y0, v_x, v_y, N,
max_time, tau,A, B, C, D, delta_t, high_y, low_y );

            if ( distance_y> distance_current_agent){
                for(int j = 0; j < 10; j++){
                    if (j <5 and abs(y[j]) <= 5 - D ){
                        population[j][i] = y[j];
                    }
                    if (j >= 5 and abs(y[j])<= 3 - D ){
                        population[j][i] = y[j];
                    }

                }
            }
        }
        t += 1;
    }

    double distance = -1;
    vector <double> best_agent(10);
    for (int i = 0; i < NP; i++ ){
        vector <double> agent(10);
        for(int j = 0; j < 10; j++){
            agent[j] = population[j][i];
        }
        double cur_dist = f(agent, x0, x,y, v_x0,v_y0, v_x, v_y, N,  max_time, tau,A, B, C, D,
delta_t, high_y, low_y );
        if(  cur_dist > distance ){
            for(int j = 0; j < 10; j++){
                best_agent[j] = agent[j];
            }
        }
    }

    return best_agent;
}

double f(vector <double> agent,
        vector <double> x0,
        vector <double> x,
        vector <double> y,
        vector <double> v_x0,
        vector <double> v_y0,
        vector <double> v_x,
        vector <double> v_y,
        int N,
        int max_time,
        double tau,
        double A,
        double B,
        double C,
        double D,
        double delta_t,
        double high_y,
        double low_y){

    // create obstacles
    vector <double> o_x (5);
    vector <double> o_y (5);


    for (int i = 0; i < 5 ; i++){
            o_x[i] = agent[i];
  }
    for (int i = 0; i < 5 ; i++){
            o_y[i] = agent[i];
  }

    // initialise force

    vector <double> F_i (2);

    for (int time = 0; time < max_time ; time++){
        for(int i = 0;  i < N; i++){
            F_i   = compute_F_i(tau, N, A, B, C, D, i, v_x0, v_y0, x, y, v_x, v_y, o_x, o_y);
            double F_i_x = F_i[0];
            double F_i_y = F_i[1];
            x[i] += v_x[i]*delta_t;
            y[i] += v_y[i]*delta_t;
            v_x[i] += F_i_x*delta_t;
            v_y[i] += F_i_y*delta_t;

            if (y[i]>high_y){
                y[i] = high_y;
                }
            if (y[i]<low_y){
                y[i] = low_y;
            }
        }
    }
    double distance = 0;
    distance = average_x_displacement(x, x0);
    return distance;
}
```



We indeed obtain an average horizontal displacement larger than if the obstacles were in a random configuration.

Question 3 : Optimal atoms configuration

In [260…

```
def energy(x):
    E = 0
    n = len(x) // 3
    x = x.reshape((n,3))
    dx = np.subtract.outer(x[:,0], x[:,0])
    dy = np.subtract.outer(x[:,1], x[:,1])
    dz = np.subtract.outer(x[:,2], x[:,2])
    r2 = dx**2 + dy**2 + dz**2
    np.fill_diagonal(r2, 1) # fill diagonal with non zero to avoid division by zero
    r6inv = r2**(-3)
    r12inv = r6inv**2
    E = r12inv - r6inv
    np.fill_diagonal(E, 0)
    return 2 * np.sum(E)

def jac(x):
    m = len(x)
    F = [0] * m
    for i in range(0, m, 3):
        for j in range(i + 3, m, 3):
            dx = x[i] - x[j]
            dy = x[i + 1] - x[j + 1]
            dz = x[i + 2] - x[j + 2]
            r2 = dx**2 + dy**2 + dz**2
            if r2 != 0:
                r2inv = 1 / r2
                r4inv = r2inv * r2inv
                r8inv = r4inv * r4inv
                r14inv = r8inv * r4inv * r2inv
                f = 24 * r8inv - 48 * r14inv
                fx = dx * f
                fy = dy * f
                fz = dz * f
                F[i] += fx
                F[i + 1] += fy
                F[i + 2] += fz
                F[j] -= fx
                F[j + 1] -= fy
                F[j + 2] -= fz
    return np.array(F, dtype = float)
```

Gradient Descent Implementation

In [332…

```
def gradient_descent(X, alpha = 0.001, eps = eps, max_iter = max_iter):
    start = time.time()
    new = 0
    R = X.copy()
    old = 10
    ite  = 0
    while abs(old - new) > eps and ite < max_iter:
        old = energy(R)
        R -= alpha*jac(R)
        new = energy(R)
        ite += 1
    end = time.time()
    return R
```

(1 + N) Evolution Srategy Optimisation

In [333…

```
def plot(X_final, name):
    "generates a 3D scatter plot of our atoms' positions "
    fig =plt.figure(figsize=(10,10))
    ax = fig.add_subplot(projection='3d')

    m = len(X_final)
    X = [X_final[i] for i in range(0, m, 3)]
    Y = [X_final[i] for i in range(1, m, 3)]
    Z = [X_final[i] for i in range(2, m, 3)]
    for i in range(len(X)):
        xs = X[i]
        ys = Y[i]
        zs = Z[i]
        ax.scatter(xs, ys, zs, color = 'b')

    ax.set_xlabel('X', fontsize = 20)
    ax.set_ylabel('Y', fontsize = 20)
    ax.set_zlabel('Z',  fontsize = 20)
    ax.set_title(f'Optimal Configuration for N = {len(X_final)//3}',  fontsize = 20)
    plt.savefig(name)
    plt.show()

def make_children(parent, sigma):
    children = []
    for i in range(len(parent)):
        children.append(np.random.normal(loc=parent, scale=sigma))
    return children

def adapt_sigma(sigma, success_ratio, boundlength):
    threshold = 0.01*boundlength
    if success_ratio > 0.2: # 1/5th rule
        sigma *= 1.2
    else:
        sigma *= 0.8

    if sigma < threshold :
        sigma=0.5*boundlength
    return sigma
```

In [334…

```
def ES_1_N(X, max_iter, eps):
    xbounds = [-1, 1]; ybounds = [-1, 1];zbounds = [-1,1]
    boundlength = max((xbounds[1]-xbounds[0]),(ybounds[1]-ybounds[0]), (zbounds[1]-zboun

    parent = X.copy()

    new, ite, success = 0, 0, 0
    sigma, adapt_every = 0.1, 5
    max_generations = max_iter
    old, new = 10, 0

    for gen in range(max_generations):
        old = energy(X)
        if abs(old - new) < eps:
            print('breaking !')
            break

        children = make_children(parent, sigma)

        Fp = energy(parent)
        Fc = [energy(child) for child in children]
        ibest = np.argmin(Fc)
        new_parent = children[ibest]

        if Fc[ibest] < Fp:
            parent = new_parent
            success += 1

        if gen % adapt_every == 0:
            success_ratio = success / adapt_every
            sigma = adapt_sigma(sigma, success_ratio, boundlength)
            success = 0
        ite += 1

    return parent
```

In [335…

```
eps_s = 1e-3
max_iter = 5000
alpha = 0.005
eps_g = 1e-15
mini = {2: -1, 3: -3, 5: -9.103852, 8:-19.821489, 16: -56.815742, 32: -139.635524, 38: -
stoch_energies = []
stoch_positions = []
grad_energies = []
grad_positions = []
```

Comparing both methods

In the cell here-under, we run the gradients descent and stochastic optimizatic techniques 5 times for each set of randomly generated N atoms for N in $[2, 3, 5, 8, 16, 32, 38]$, and keep the best score. We then keep the best performances of our gradient and stochastic based algorithms and plot them.

In [336…

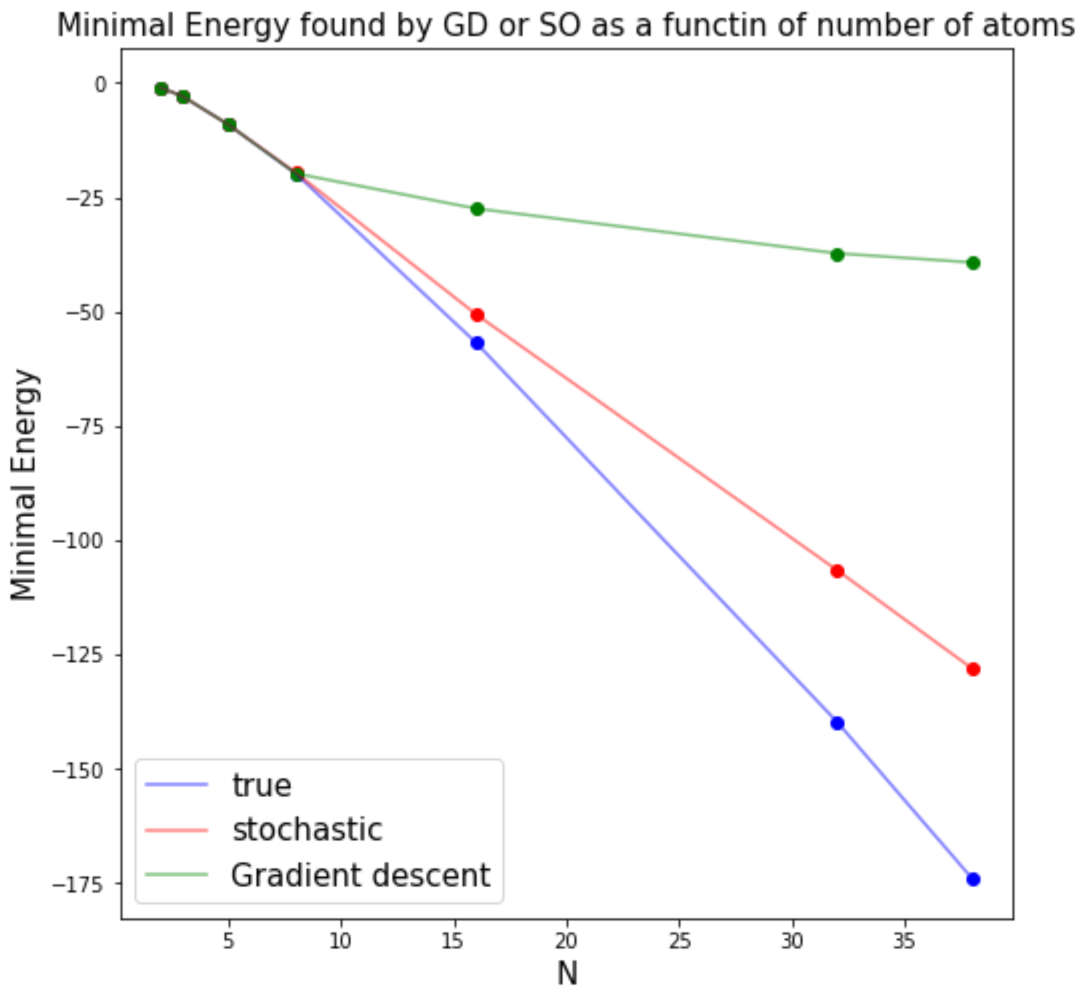
```
Ns = [2, 3, 5, 8, 16, 32, 38]
tries= 5

for N in Ns:
    print(f'N = {N}')
    print(f'   True minimum : {mini[N]}')
    grad_energy = []
    grad_pos = []

    stoch_energy = []
    stoch_pos = []
    for i in range(tries):
        X = np.random.normal(-1,1, size = 3*N).reshape(-1,1)
        X_G = gradient_descent(X, alpha = alpha, eps = eps_g, max_iter = max_iter)
        e_g = energy(X_G)
        print(f'   Gradient Descent : {e_g}')
        grad_energy.append(e_g)
        grad_pos.append(X_G)

        X_S = ES_1_N(X, eps = eps_s, max_iter = max_iter)
        e_s = energy(X_S)
        print(f'   Stochastic Optimization : {e_s}\n')
        stoch_energy.append(e_s)
        stoch_pos.append(X_S)

    grad_energies.append(min(grad_energy))
    grad_positions.append(grad_pos[np.argmin(e_g)])

    stoch_energies.append(min(stoch_energy))
    stoch_positions.append(stoch_pos[np.argmin(stoch_energy)])
```

```
N = 2
   True minimum : -1
   Gradient Descent : -0.0009291502694511207
breaking !
   Stochastic Optimization : -0.0008438354361489721

   Gradient Descent : -0.9999999999999999
   Stochastic Optimization : -0.9999999952437784

   Gradient Descent : -0.9999999999999998
   Stochastic Optimization : -0.999999999997338

   Gradient Descent : -0.9999999999999999
   Stochastic Optimization : -0.9999999999783946

   Gradient Descent : -0.0017486336083486365
   Stochastic Optimization : -0.9999999947195202

N = 3
   True minimum : -3
   Gradient Descent : -3.0
   Stochastic Optimization : -2.9998236671905296

   Gradient Descent : -2.9999999999999996
   Stochastic Optimization : -2.9998729898421903

   Gradient Descent : -3.0
   Stochastic Optimization : -2.999857904658799

   Gradient Descent : -3.0
   Stochastic Optimization : -2.999803203723241

   Gradient Descent : -3.0
   Stochastic Optimization : -2.9996503705904525

N = 5
   True minimum : -9.103852
   Gradient Descent : -3.0000007881606554
   Stochastic Optimization : -9.074122781694047
   Gradient Descent : -3.0
   Stochastic Optimization : -6.007915754310855

   Gradient Descent : -9.103852415707554
   Stochastic Optimization : -9.09416365744098

   Gradient Descent : -9.103852415707557
   Stochastic Optimization : -9.082012310009347

   Gradient Descent : -6.000939246106917
   Stochastic Optimization : -5.995667782386376

N = 8
   True minimum : -19.821489
   Gradient Descent : -12.30292804835786
   Stochastic Optimization : -13.847809396597848

   Gradient Descent : -6.000125941458016
   Stochastic Optimization : -19.025651104407075

   Gradient Descent : -18.85682616777114
   Stochastic Optimization : -19.630972290038677

   Gradient Descent : -12.30292752958072
   Stochastic Optimization : -17.458395130972505

   Gradient Descent : -19.821489192154743
   Stochastic Optimization : -13.317419653967

N = 16
   True minimum : -56.815742
   Gradient Descent : -27.479751195511504
   Stochastic Optimization : -45.6186942541417

   Gradient Descent : -12.30475093312776
   Stochastic Optimization : -43.146752751022774

   Gradient Descent : -18.835658000036222
   Stochastic Optimization : -38.31039782982794

   Gradient Descent : -15.596293242125206
   Stochastic Optimization : -50.58404438690185

   Gradient Descent : -25.916875849465526
   Stochastic Optimization : -33.090261908817155

N = 32
   True minimum : -139.635524
   Gradient Descent : -19.82149054469367
   Stochastic Optimization : -101.62421806843308

   Gradient Descent : -37.2623592231632
   Stochastic Optimization : -90.64897342712193

   Gradient Descent : -31.907165966914793
   Stochastic Optimization : -82.48312734854966

   Gradient Descent : -15.593338138572342
   Stochastic Optimization : -106.49631558663768

   Gradient Descent : -33.06437471335289
   Stochastic Optimization : -98.43719805118286

N = 38
   True minimum : -173.92842651178944
```

```
Gradient Descent : -35.161401245194135
Stochastic Optimization : -121.28505447174943

Gradient Descent : -22.083731084153744
Stochastic Optimization : -120.70933992071082

Gradient Descent : -23.19759237670327
Stochastic Optimization : -114.43516419015678

Gradient Descent : -39.251236281040114
Stochastic Optimization : -128.01079498489463

Gradient Descent : -9.131116640896757
Stochastic Optimization : -120.9045660435648
```

In [337…

```
fig =plt.figure(figsize=(8,8))
plt.plot(Ns, list(mini.values()),alpha = 0.5, c = 'b', label = 'true')
plt.plot(Ns, stoch_energies, c = 'r',alpha = 0.5, label = 'stochastic')
plt.plot(Ns, grad_energies, c  = 'g',alpha = 0.5, label = 'Gradient descent')
plt.scatter(Ns, list(mini.values()), c = 'b')
plt.scatter(Ns, stoch_energies, c = 'r')
plt.scatter(Ns, grad_energies, c  = 'g')
plt.legend(loc = 'lower left', fontsize = 15)
plt.xlabel('N', fontsize = 15)
plt.ylabel('Minimal Energy', fontsize =15)
plt.title('Minimal Energy found by GD or SO as a functin of number of atoms', fontsize =
plt.savefig(f'SO_vs_GD_{5}_tries')
plt.show()
```



We can see that for a 'low' number of atoms (N = 2, 3, 5, 8), stochastic and gradient based method manage to find an optimal configuration having a potential energy almost equal to the known minimum potential energy.

```
In [343…
print('Theoretical minimum energy for N = 2 is : ', mini[2])
print('Minimum Energy found for N = 2 with a gradient based method  is :', grad_energies
print('Minimum Energy found for N = 2 with a stochastic method  is :', stoch_energies[0]
print('\n')
print('Theoretical minimum energy for N = 3 is : ', mini[3])
print('Minimum Energy found for N = 3 with a gradient based method  is :', grad_energies
print('Minimum Energy found for N = 3 with a stochastic method  is :', stoch_energies[1]
print('\n')
print('Theoretical minimum energy for N = 5 is : ', mini[5])
print('Minimum Energy found for N = 5 with a gradient based method  is :', grad_energies
print('Minimum Energy found for N = 5 with a stochastic method  is :', stoch_energies[2]
print('\n')
print('Theoretical minimum energy for N = 8 is : ', mini[8])
print('Minimum Energy found for N = 8 with a gradient based method  is :', grad_energies
print('Minimum Energy found for N = 8 with a stochastic method  is :', stoch_energies[3]
```

```
Theoretical minimum energy for N = 2 is :  -1
Minimum Energy found for N = 2 with a gradient based method  is : -0.9999999999999999
Minimum Energy found for N = 2 with a stochastic method  is : -0.999999999997338


Theoretical minimum energy for N = 3 is :  -3
Minimum Energy found for N = 3 with a gradient based method  is : -3.0
Minimum Energy found for N = 3 with a stochastic method  is : -2.9998729898421903


Theoretical minimum energy for N = 5 is :  -9.103852
Minimum Energy found for N = 5 with a gradient based method  is : -9.103852415707557
Minimum Energy found for N = 5 with a stochastic method  is : -9.09416365744098


Theoretical minimum energy for N = 8 is :  -19.821489
Minimum Energy found for N = 8 with a gradient based method  is : -19.821489192154743
Minimum Energy found for N = 8 with a stochastic method  is : -19.630972290038677
```

However, as the number of atoms increases, we can see that our gradient based method reaches its limit and falls into local minima of low number of atoms. Indeed, we can see that for N = 16, 32 and 38, our gradient based method can't find significantly better configurations than the N = 16 or 32 atoms system. This is not the case for our $1 + N$ stochastic evolution strategy which manages to find better configurations than the gradient based method for high number of atoms. Indeed, it manages to find an optimal configuration with a potential energy of -128 J for N = 38 atoms, when the theoretical minima is around -173.92842651178944J.

We note that we can have different optimal configurations for our N particles giving the same minimal energy. Indeed, simpliy rotating our atoms along the z-axis will not change the overal potential energy of our system. In other words, there is an infinite amount of solutions that give a global minima for our potential energy.

```
In [ ]:
```