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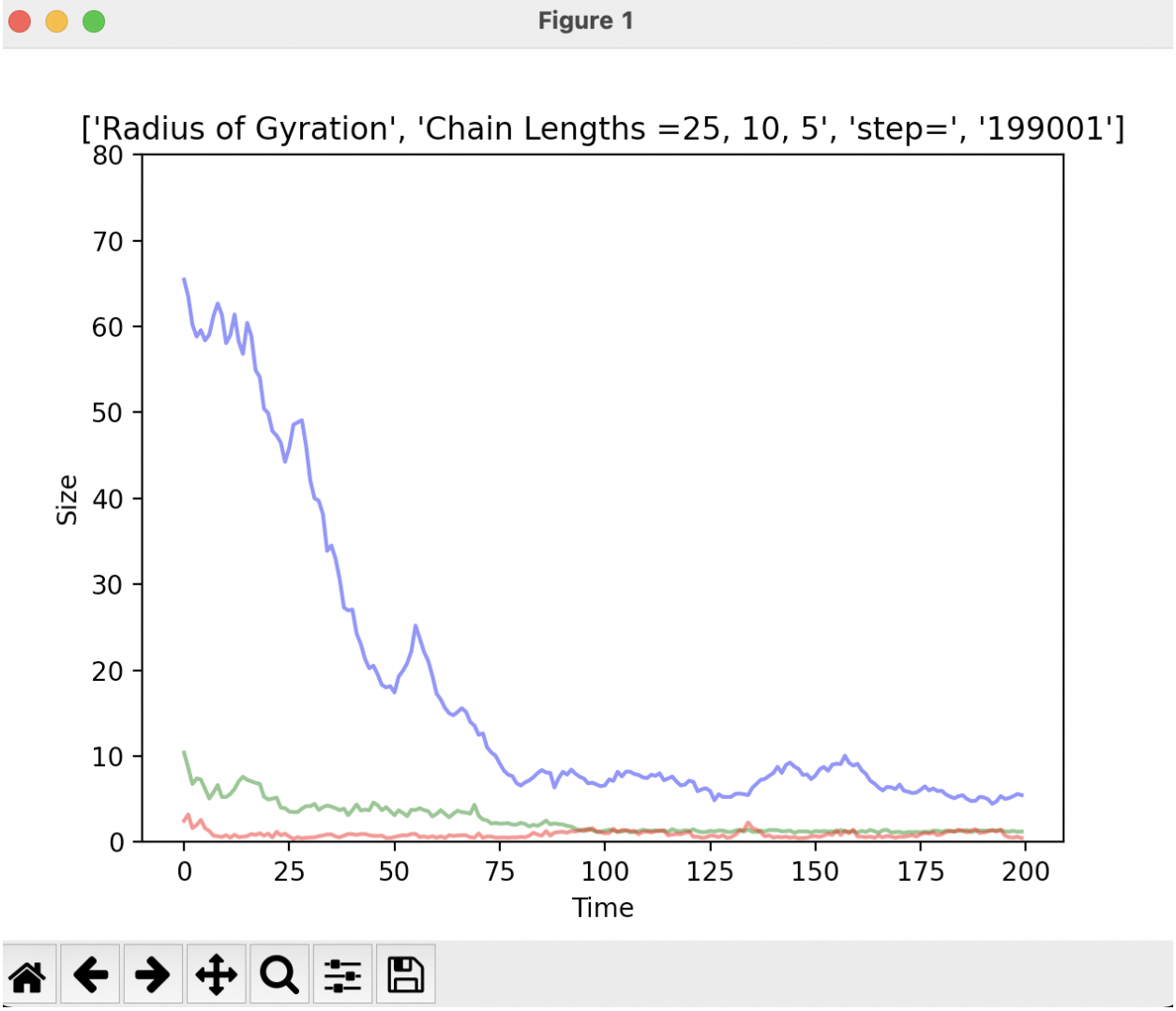
CSCI4314

Part 1: Protein Folding

(1) Plot of Radius of Gyration for different chain lengths over 200,000 time steps



Key

Blue	*Chain Length N = 25*
Green	*Chain Length N = 10*
Red	*Chain Length N = 5*

Algorithm:

```
def radius_gyration_size(N, x):

  #25 x,y coordinates for each instance of the simulation: 200000/1000 simulations
   sum = 0
   for i in range(N):
       for j in range(N):
           if i!=j:
               #summing distance between amino acid i and j with distance formula
               #(ri - rj)^2
               #x[i,:]
               diff = x[i,:] - x[j,:]
               #print(f"diff: {diff}")
               sum += (diff[0] - diff[1])**2


   return sum/(2* (N**2))
```

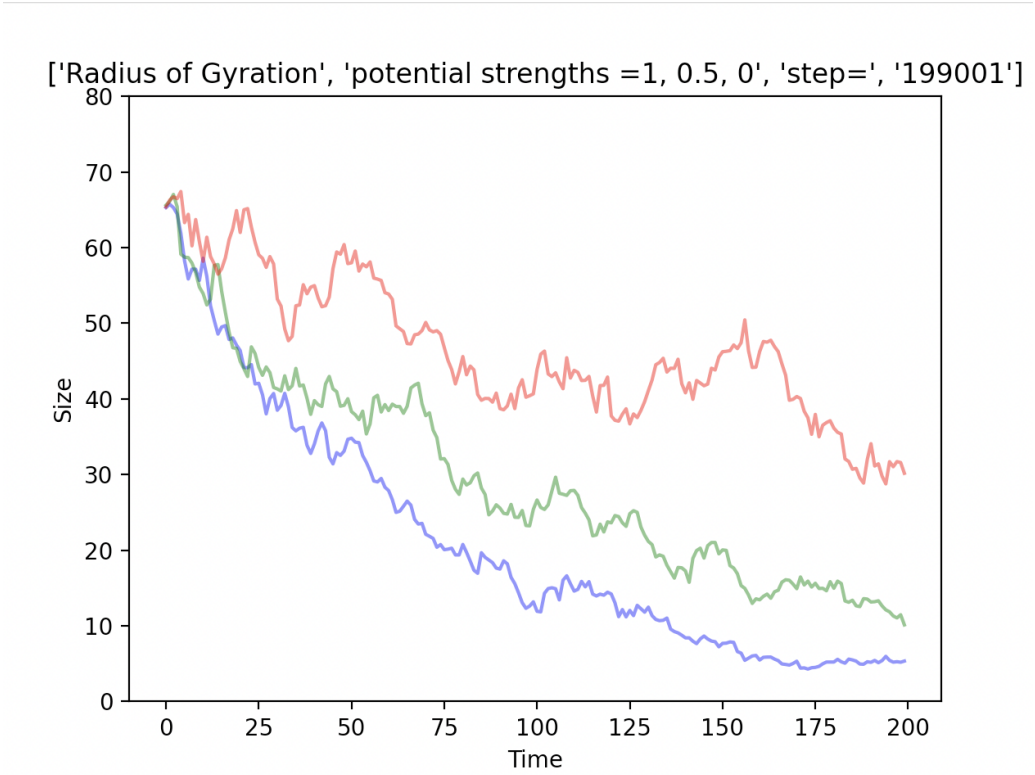
Calling the routine:

```
   lengths = [25,10,5]
   arrays = [[],[], []]
   for index, len in enumerate(lengths):
       x = initial_configuration(min_sep, len)
       for step_i in range(0, step_gyration): #molecular dynamics loop
           #motion - position of next time step
           x, pairs = steepest_descent(len, x, dt, cutff_LJ, epsilon_LJ, min_sep,
spring_coeff, T)
           #returns a size

           if (np.mod(step_i-1,print_interval) == 0):  #print every 1000 steps
               arrays[index].append(radius_gyration_size(len, x))


               mytitle = ["Radius of Gyration",  "Chain Lengths =25, 10, 5", "step=",
str(step_i)]

               print(mytitle)
   visualize_size(N, arrays[0], arrays[1], arrays[2],  pairs, mytitle)
```

Visualizing the output:

```
def visualize_size(N, size_25, size_10, size_5, pairs, mytitle):

    plt.ylim(top=80,bottom=0)
    plt.plot(size_25, color = 'blue', alpha=0.5, label = "N=25")
    plt.plot(size_10, color = 'green', alpha=0.5, label = "N=10")
    plt.plot(size_5, color='red', alpha=0.5, label = "N = 5")
    plt.title(mytitle)
    plt.xlabel("Time")
    plt.ylabel("Size")
    plt.show()
    Return
```

(2) Plot of Radius of Gyration for Different LJ strength potentials



Key

Blue	*LJ Potential Strength = 1*
Green	*LJ Potential Strength = 0.5*
Red	*LJ Potential Strength = 0*

Calling routine:

```
   epsilon_LJ=[1, 0.5, 0]
   radius = [[],[],[]]
   for index, e in enumerate(epsilon_LJ):
       x = initial_configuration(min_sep, N)
       for step_i in range(0, step_gyration): #molecular dynamics loop
           #motion - position of next time step
           x, pairs = steepest_descent(N, x, dt, cutff_LJ, e, min_sep, spring_coeff,
T)
           #returns a size

           if (np.mod(step_i-1,print_interval) == 0):  #print every 1000 steps
               radius[index].append(radius_gyration_size(N, x))



               mytitle = ["Radius of Gyration",  "potential strengths =1, 0.5, 0",
"step=", str(step_i)]

               print(mytitle)
               #we need pairs
               #visualize size over 200000 time steps for sizes 25,10,5


   visualize_lj(N, radius[0], radius[1], radius[2],pairs, mytitle)
```

Part 2: Paper Review

Review of Design and self-assembly of two-dimensional DNA crystals

1. **What do you feel the main contribution of this paper is? (10 points)**

Dr. Eric Winfree and his team provide scientists with the insight needed to design and create self-assembling periodic (crystal) DNA matter. The paper highlights the importance of branched DNA with programmable sticky ends, which make for good molecular crystal design. In order to create specific periodic patterns, as mentioned in the abstract, the use of anti-parallel double crossover (DX) DNA enables predictable and controllable interactions. These design aspects that Winfree discusses will be suitable for the assembly of periodic matter because of its rigidity, and this knowledge is a great contribution to the scientific field and those that conduct research in molecular structures.

Winfree utilizes programmable tiles that can interact with each other and these are used to model DX molecules and their assembly. The program will mimic a Turing Machine as an algorithm to create specific lattice structures. Even more so, the scalability of this design is incredible as it can create structures at the nanometre scale. It is evident that the applications of computer science and computational biology are of increasing importance and interest within the scientific community.

Moreover, this paper illustrates that the team's ability to successfully create self-assembling AB lattice structures, using their DX method with sticky-ends, indicates that this design method coupled with automata can lead to the creation of other self-assembling molecular structures that may be useful in nanotechnology and computation. This contribution is imperative to solve future health problems, environmental issues, and computational problems.

2. **What's the essential principle that the paper exploits? (10 points)**

The essential principle that this paper exploits is the application of self-assembling structures in nanotechnology and the efficacy of rigid, double-crossover helixes in the design. Winfree shows that the methods used to create their AB lattice can be applied to the creation of these structures and how a bottom-up approach can be used to achieve desired results.

3. **Describe one major strength of the paper. (10 points)**

This paper does an excellent job of connecting the methods that they used to create self-assembling molecules to the premise of the research. For example, the introduction of the paper describes how antiparallel double-crossover structures are useful for the formation of

precise, controlled structures. The researchers use this design method to construct their own models using Wong tiles, which shows consistency and authenticity in their research.

4. **Describe weakness of the paper. (10 points)**

This paper could have highlighted how future works could use their research in order to improve models involving nanogold particles, which is something that this paper lacked information on. Continued testing with these different chemical groups will allow researchers to understand how different solutions can affect the interaction of sticky-end DX structures.

5. **Describe one future work direction you think should be followed. (10 points)**

As indicated in the applications section of the paper, future work that can follow this research might entail the crystallization of self-assembling macromolecules. The structures can be used to create molecular electronic components or biochips which will help medical facilities manage their patients more efficiently.