MODELING A NANODIMER IN A LIQUID USING STOCHASTIC ROTATION DYNAMICS

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Abstract. In this project, I will be simulating the time evolution of a liquid composed of two distinct species with dissolved nanodimers. The species will repulse the nanodimer once they get close, but the magnitude of repulsion will be different between species. There will also be a chemical reaction from one species to another when the species are in close contact to the nanodimer. The interacting forces of the liquid particles will be modeled by a periodic averaging of the directions of particles close to one another, resulting in "clumps" of the particles moving together. We will be primarily interested with the composition of the liquid and the motion of the nanodimer. Nanodimers that are chained together will possibly be included. The simultion will be done computationally using code handwritten in C and ported from different languages into C.

1. Implementation

The main advantage of stochastic rotation dynamics over other liquid modeling algorithms is simplicity of coding. First, periodic boundaries are imposed on the system, which is broken up into a grid. Each grid square has a side length of 1. This grid exists in order to simulate the localized nature of liquid interactions.

The entire algorithm consists of two steps, the streaming step:

$$r_i(t+\tau) = r_i(t) + \tau * v_i(t) \tag{1}$$

and the collision step:

$$v_i(t+\tau) = U(t, r_i(t)) + R(\omega(r_i(t))) * (U(t, r_i(t)) - v_i(t)) \tag{2}$$

applied to every particle at each time step, where $r_i(t)$ and $v_i(t)$ are the position and velocity of the i^{th} particle at time t, $/tau$ is the time step, $U(t, r_i(t))$ is the average velocity of the particles in the grid square to which r_i belongs at time t, and $R(\omega(r_i(t)))$ is the rotation matrix corresponding to the grid square to which r_i belongs at time t. The streaming step is a simple application of Eulers time step algorithm for solving differential equations, and the collision step is meant to simulate the interactive forces between all particles in a given grid square. In the collision step, the average velocity of all particles in a grid cell is calculated, and then the difference of the velocity of the particle and the average velocity of all particles in its grid square is taken. The vector resulting from this difference is rotated by a pre-defined angle, and the result is added to the average velocity of the particles in the grid square to give the new velocity for the particle. The only particles that interact with a given particle in this matter are the particles in the same grid square. The rotation angle can vary from grid square to grid square,

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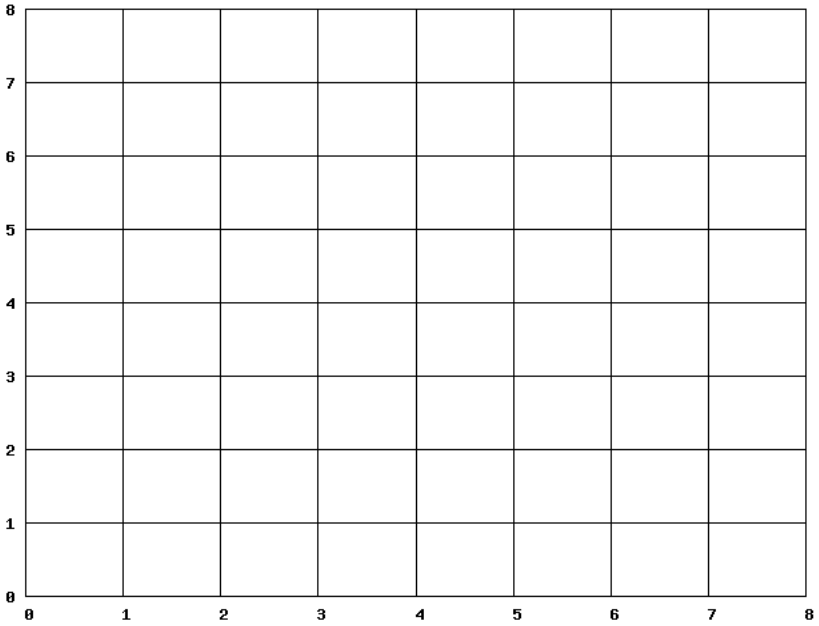

FIGURE 1. An example of the discretation of the grid.

but in the present application the absolute value of the rotation angle is the same throughout the system, and the sign of the rotation angle is randomly chosen at the beginning of the simulation. The rotation angle determines the degree to which the particle interact with each other; at a rotation angle of 0 there is no interaction but at a rotation angle of 90 degrees there is strong interaction.

Into this liquid is inserted a polymer. The polymer is modeled as multiple particles with each particle connected to two other particles by springs obeying Hookes law,

$$\frac{d^2r}{dt^2} = -k(r-L) \tag{3}$$

where r is the length of the spring connecting the particles, L is the equilibrium length of the spring, and k is constant for the spring. Each particle in the polymer interacts with the liquid close to the polymer, which is modeled by having a distance associated with each particle in the polymer. Any liquid particle that is within this distance of a polymer particle will interact with the polymer using a standard inverse square repulsive force,

$$\frac{d^2r}{dt^2} = \frac{k}{r^2} \tag{4}$$

where r is the distance between the liquid particle and the polymer particle and k is a constant that depends on the liquid particle. Each liquid particle belongs to one of two species, A or B. Both species interact with each other normally in stochastic rotation dynamics, but they interact differently with the polymer. How they interact

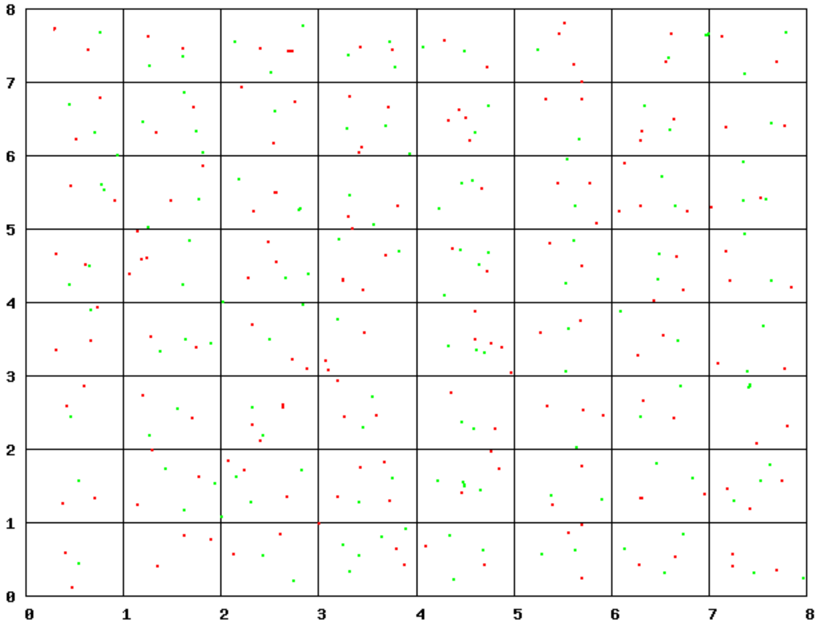

FIGURE 2. The liquid particles. The different colors correspond to different liquid particle type, which is not relevant for stochastic rotation dynamics but will become important with the introduction of the dimer.

differently is determined by the constant k in the inverse square repulsive force. Finally, each polymer particle has a chance to convert either particles of species A into species B or particles of species B into species A. Each polymer particle can only convert the particles one way, so that after a long period of time each polymer particle will have one species of liquid predominately clustered around it.

So why is this being done? Consider a dimer, a polymer with only two particles, and suppose that the left particle converts A to B and the right converts B to A. Suppose also that B particles react more strongly with the polymer than do A particles. Over time, near the left particle there will be an accumulation of B particles and near the right particle there will be an accumulation of A particles. However, because the liquid particles and the polymer particles are repulsive, the liquid particles will be pushed away from the polymer particles. Thus, many A particles will be repulsed away from the right polymer particle and towards the left polymer particle, and many B particles will be repulsed away from the left polymer particle and towards the right polymer particle. Not only that, but since B particles react more strongly with the polymer than do A particles, there will be more B particles being repulsed, and they will be moving faster. So there will be a net surplus of B particles coming in on the right polymer particle from the left, and a net surplus of A particles coming in on the left polymer particle from the right. However, these two surplus will not cancel each other out with respect to the total force on the polymer, since the B particles react more strongly than do the A

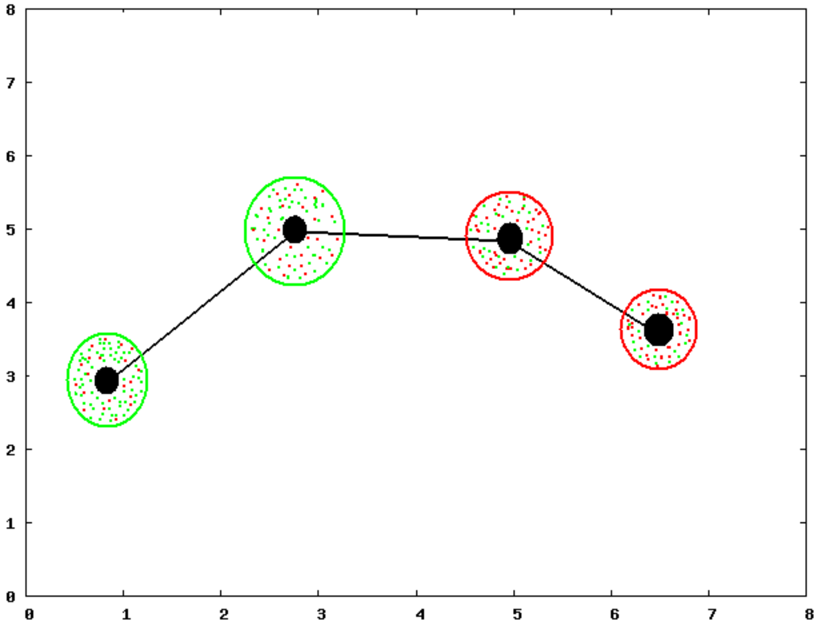

Figure 3. The dimers and their radii of interaction with the liquid. Note that the size of the polymer particles are exaggerated for demonstrational purposes, the actual particles are point particles like the liquid particles. The circles around each particle demonstrate the region of space where the polymers and the liquid interacts. Only the liquid particles near the polymer particles are shown.

particles. Thus it is feasible that the polymer will move to the right over time, as the influx of B particles dominates the influx of A particles. Due to this imbalance and the different in repulsive force of the two liquid particles species, propulsion is expected to be observed moving along the dimer axis.

The direction and magnitude of this propulsion depends on the interactivity between the liquid species and the dimer, for as B particles become more reactive with the dimer, we expect to see the B particles dominating the propulsion of the dimer as well as increasing the magnitude of the propulsion. Because there are forces causing a torque in the dimer, there will be rotation of the dimer, so simply plotting the course of the dimer molecules is not useful for determining whether propulsion occurs. In addition, the dimer may be subject to temporary uneven influxes of particles from outside the radii of interaction, leading to periods of rapid change in the propulsion of the dimer. Thus, the best way to determine if propulsion is occuring is to take the time average of the propulsion of the dimer. This is done by calculating the center of mass velocity of the dimer, then taking the projection of this velocity along the dimer axis to obtain the instantaneous propulsion velocity. Adding all the propulsion velocities from time step 0 to time step i and dividing by i+1 yields the time average for the propulsion velocity at

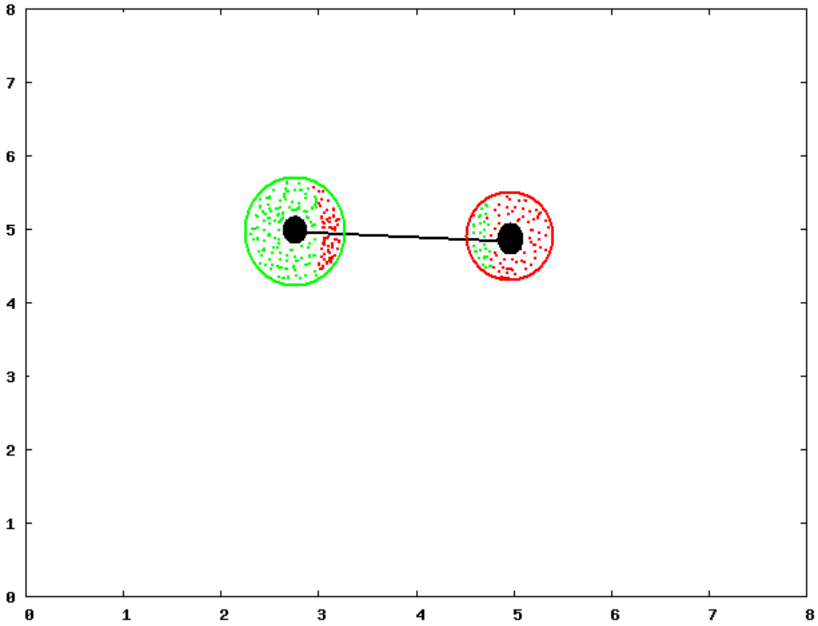

Figure 4. A dimer with an inbalance of A and B particles near its constituent particles. This imbalance is expected to produce propulsion.

time step i. Should the system relax into a steady state, for large values of i the time average of propulsion velocity should be constant, which implies an essentially constant propulsion velocity for the dimer. This is the measure of the propulsion of the system. It is the intent of my project that I will be able to be able to observe this phenomena computationally.

2. Results

The results are currently less than satisfactory. Individually, each section of the program works. However, we are not observing a stable state in the propulsion of the dimer. This might be due to the fact that the time it takes to reach a stationary state is longer than the time frame of one hundrend seconds. Furthermore, despite expectations that the magnitude of the dimer propulsion will increase as the ratio between A and B's force constants increase, there is no corrolation between the two. Although for equal force constants the propulsion is zero (as to be expected), as the force constants increase the rough value for the dimer propulsion jumps in a seemingly random order. This might be due to the fact that the force varies rapidly to infinite close to the dimer particles, combined with the fact that the algorithm has a streaming step which is essentially an Euler integration scheme, which has low tolerance to error. It is planned in the future that we wil move to a Hooke's Law force, which varies very slowly and thus suffer less from error in small distances. More work needs to be done in this topic before publishable data can be obtained.

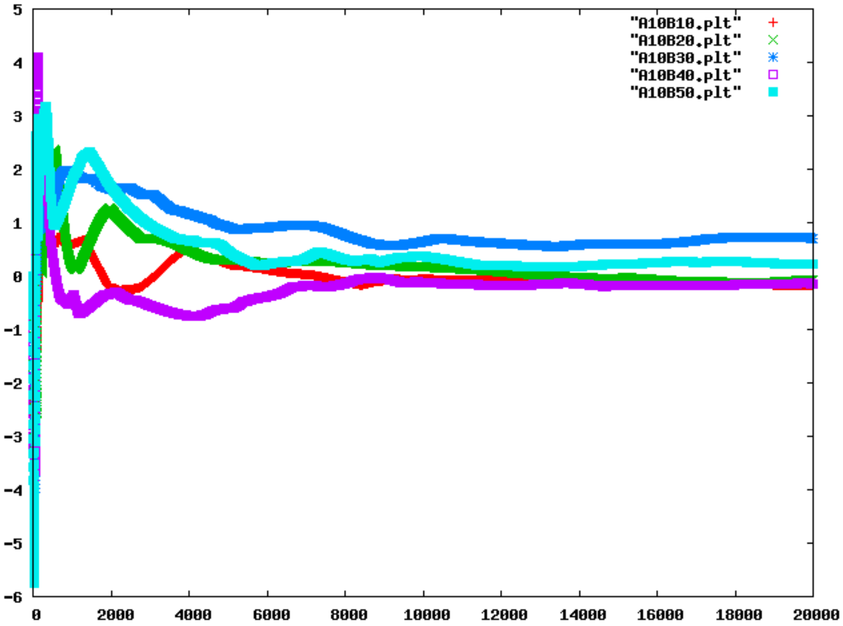

Figure 5. A graph of the running time average of the dimer propulsion velocity. Different lines correspond to different force constant ratios.

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