Problem Set 5

Biological Physics

Due Thurs., April 21, 2015

The Vicsek Model and the Radial Distribution Function

For this problem set, you will modify the Vicsek model assigned in class to include a repulsive force to prevent particle overlaps, and investigate the radial distribution function $g(r)$ and the order parameter $\langle\phi\rangle_t$ for the two models.

A) Adding Repulsion

Download `lecture18 / vicsekvelocity.m` and `lecture18 / vicseklooper.m` from the classesv2 server.

Currently, the `vicsekvelocity` models the "standard" Vicsek model:

$$\vec{v}_i(t+\Delta t) = v_0 \vartheta\left(\sum_{j\in S_i} \vec{v}_j(t) + \eta |S_i| \vec{\xi}_i\right)$$

where $\vartheta(\vec{x}) = \hat{x} = \frac{\vec{x}}{|x|}$ is a normalizing function, S_i is the set of particles such that $|\vec{r}_{ij}| < r_0$, $|S_i|$ is the number of particles such that $|\vec{r}_{ij}| < r_0$, $\vec{\xi}$ is a random unit vector, there is a density $\rho = \frac{N}{L^2}$, L is the size of the box, and v_0, r_0, and η are parameters.

We are going to modify this equation to add in a repulsive force:

$$\vec{v}_i(t+\Delta t) = v_0 \vartheta\left(\sum_{j\in S_i} \vec{v}_j(t) + \beta \sum_{j\in S_i} \vec{f}_{ij} + \eta |S_i| \vec{\xi}_i\right)$$

$$\vec{f}_{ij} = \begin{cases} \left(1 - \frac{r_{ij}}{r_c}\right)\hat{r}_{ij} & r_{ij} < r_c \\ 0 & r_{ij} > r_c \end{cases}$$

1. Add two parameters to the `vicsekvelocity` function, `beta` and `rc`.

2. Modify the body of this function to account for this repulsive force. Note that this can be done with a couple simple array indexing and mathematical operations inside the `for i=1:N` loop.

3. **[Output]** Calculate $\langle\phi\rangle_t$ for $0.5 \leq \eta \leq 0.7$ (`etas = 0.50:0.02:0.7`) for $\beta = 0$ and $\beta = 100$, and plot $\langle\phi\rangle_t$ vs. η for both values on the same graph. Use a legend to indicate which is which.

   Use the parameters $\Delta t =$ `dt` $= 0.1$, $r_0 =$ `r0` $= 1$, $r_c =$ `rc` $= 0.1$, $\rho =$ `rho` $= 1.5$, $v_0 =$ `v0` $= 0.5$, and $L = 6$.

4. **[Output]** Approximate roughly (i.e., just eyeball) the value of η_t, where $\langle\phi\rangle \approx 0.5$ for the two models. Does it increase or decrease when repulsion is added?

A) Calculating the Radial Distribution Function

1. Modify the `vicsekvelocity` function to return two values:

   ```
   function [fs, rijdists] = vicsekvelocity(v0, r0, rc, eta, beta, L, rs, vs)
   ```

   where `rijdists` is an $N \times N$ matrix of $|\vec{r}_{ij}|$ values. Note that most of this is already done for you in the `for i=1:N` loop; you just need to create an empty matrix before the loop and then fill it with the correct values during the loop.

2. At every step, calculate a histogram of $|\vec{r}_{ij}|$ distances, and sum these histograms over all steps to get $n(r, r+\delta)$ like we did in class. See `classesv2 / lecture17` for code examples on how to do this. Note that you will need to throw away values where $|\vec{r}_{ij}| = 0$ (that is, don't count $|\vec{r}_{ii}|$) and where $\vec{r}_{ij} \geq \frac{L}{2}$.

3. Calculate the radial distribution function $g(r)$. To normalize this, remember that there are $N_{\text{steps}} N_{\text{particles}}$ "disks" summed over in $n(r, r+\delta)$, and the area of each of these disks is $a(r, r+\delta) = 2\pi r\delta$. For the ideal gas, particles would be evenly distributed, so the number of particles in each disk for the ideal gas would be $h(r, r+\delta) = 2\pi r\delta\rho$, giving us

   $$g(r) = \frac{n(r, r+\delta)}{N_{\text{steps}} N_{\text{particles}}} \frac{1}{2\pi r\delta\rho}$$

4. **[Output]** Plot $g(r)$ vs. $\frac{r}{r_c}$ for $\eta_0 = 0.2, 0.5, 0.7$ for both the standard and repulsive models. with the two models in different figures. Use the `csvread` function to read in `gr0.3.csv`, which will give you a 500×2 array of $\left(\frac{r}{\sigma}, g(r)\right)$ values for $\phi = 0.3$ for hard disks, where σ is the diameter of the hard disks, and plot this as well. Use a legend to indicate the hard sphere model and the three different η values.

Submission

As before, make a zip (or tar) file with your code in `.m` format, all your graphs in in `.eps` format, and the answers to the questions in `.txt`, `.rtf`, or `.pdf` format. Upload to the classesv2 Assignments section, *named with the format* ***`LASTNAME-FIRSTNAME-PS5.zip`*** (or `.tar` / `.tgz`).