Guo-Jun Liao
guo-jun.liao@campus.tu-berlin.de
+49 30 314 28852

Phase separation: From passive fluids to active systems

Self-propelled particles convert the energy stemming from an internal source or stored in the surroundings into their own active motion. A typical consequence is persistent motion, that is, the particle moves along a straight line up to a distance much longer than its size, even in presence of a solvent creating thermal noises. Due to this feature, active systems often exhibit remarkable collective behavior.

In this project, you will implement a code for simulating passive fluid systems and check whether the energy and pressure values are correct. Based on this code, you will further develop a code for simulating a model of active systems and observe phase separation induced by the active motion.

1. Passive Lennard-Jones fluids

You will be given a nearly completed code for simulating two-dimensional Lennard-Jones (LJ) fluids, where particles interact via the Lennard-Jones potential [1],

$$U_{LJ}(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right].$$

If you want to sharpen your programming skills, you are also encouraged to write the whole simulation code on your own. To validate the code, you should compare with the literature [2-4] several properties of the passive LJ fluids, such as the energy and pressure. You can also check the vapor-liquid phase separation of LJ fluids with suitable parameter combinations. Then, we proceed to the active systems.

2. Active Brownian particles

Through slightly modifying the code for LJ fluids, we will implement active Brownian particles, a simple yet famous model system describing purely repulsive, isotropic particles subject to a self-propulsion force. The tasks of implementation include:

(1) To change the interaction potential into a purely repulsive variant via shifting up the LJ potential. The functional form is given by

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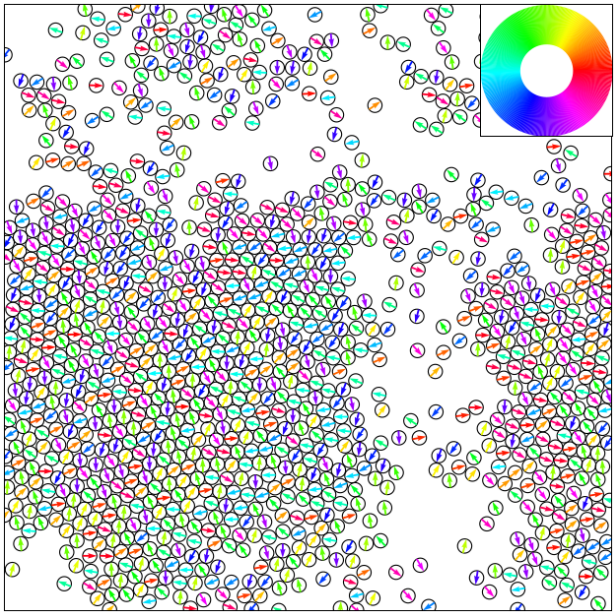
$$U(r) = \begin{cases} 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} + \frac{1}{4}\right], \text{if } r < 2^{1/6}\sigma \\ 0, \qquad\qquad \text{else.} \end{cases}$$

(2) To assign a self-propulsion force onto every particle with a constant magnitude and the direction diffusing over time.

With the increasing magnitude of the propulsion force, you will observe the motility-induced phase separation [5], in which freely moving particles coexist with close-packed dense clusters, as shown in the figure below.



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