Simulation read me

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I. ELEMENTS OF SIMULATION

The simulation is written with 3 distinct elements in mind. We have included 3 particle types:

- **Fluid A** monomers of type A
- **Fluid B** monomers of type B
- **Microtubule (MT)** Microtubule monomers

Independent of their interactions, each of the species evolves in time according to standard Langevin dynamics in an NVT ensemble with periodic boundary conditions.

II. INTERACTIONS

The interactions between all the elements in the system can be rougly characterized in terms of equilibrium and non-equilibrium interactions. We shall list the elements of each in turn

A. Equilibrium interactions

We list below all the potentials that will be used:
The Lennard Jones Potential:

$$\phi_{LJ}(r) = 4\epsilon\left(\left(\frac{\sigma}{r}\right)^1 2 - \left(\frac{\sigma}{r}\right)^6\right) \tag{1}$$

The WCA Potential:

$$\phi_{WCA}(r) = \begin{cases} 4\epsilon\left(\left(\frac{\sigma}{r}\right)^1 2 - \left(\frac{\sigma}{r}\right)^6\right) + \epsilon, & \text{if } r \leq 2^{1/6}\sigma \\ 0, & \text{otherwise} \end{cases} \tag{2}$$

The FENE potential

$$\phi_{FENE}(r) = -0.5KR_0^2 \ln\left(1 - \frac{r}{R_0}^2\right) \tag{3}$$

The Bending potential:

$$\phi_{\text{BEND}}(\theta) = 0.5k_b(\theta - \theta_0)^2 \tag{4}$$

For the equilibrium interactions we have the following:

- **Equilibrium interaction between A and A** Fluid A interacts with itself through a Lennard-Jones interaction, with a diameter σ, and attraction ϵ
- **Equilibrium interaction between B and B** Fluid A interacts with itself through the same Lennard-Jones interaction as fluid A, with a diameter σ, and attraction ϵ
- **Equilibrium interaction between A and B** Fluid A and Fluid B interact with each other through a purely hard sphere repulsion, (WCA potential with an attractive part of the interaction set to 0)

The additive effect of these interactions listed thus far is we have a parameter ϵ which will control the propensity of the fluids A and B to phase separate.
Now including the additional equilibrium interactions with the microtubule:

- **Equilibrium interaction between A and MT** The equilibirum interaction between A and MT is a purely hard sphere interaction (WCA potential with attractive part of interaction set to zero)

- **Equilibrium interaction between B and MT** The equilibirum interaction between B and MT is a purely hard sphere interaction (WCA potential with attractive part of interaction set to zero)
- **Equilibrium interaction between MT and MT** The interactions between the MT particles have two different elements. All MT monomers feel a WCA potential with each other. Additionally, MT monomers which are on the same microtubule will interact with a backbone (FENE) potential (strong penalization to extension), and a bending potential (strong potential to bending). The parameters K and k control the extent of equilibrium extension and bending modes, respectively.

This systhem thus defined would be of an equilibrium system of microtubules embedded in a binary fluid mixutre.

B. Non-equilibrium interactions

In addition to the above equilibrium elements of the simulation, we can build in non-equilibrium interactions to the previously defined elements.

Chemical dynamics between A and MT, and between B and MT The monomers A and B can bind/unbind to the microtubule. There are several distinct elements to this:

- **Binding** Binding occurs when a monomer A or B is within a distance d_{bind} (taken to be 1.2σ by default) of a monomer of MT. With a probabilty P_{bind} at each timestep of the simulation, the monomer A or B will form a bond with the microtubule monomer. This means in practice that we establish a bond between the monomer and the microtubule. The bond is given by an additional potential that is inserted into the simulation, being a harmonic potential:

$$\phi_{\mathrm{BIND}}(r) = \frac{1}{2} k_{bind}(r - r_0)^2 \tag{5}$$

  where r_0 sets the preferred distance for the monomer A or B to be from the MT, and k_{bind} sets the strength of the bond. In addition to the potential being turned on, we also track where on the microtubule the monomer A or B is bound too, and the potential is calculated using the difference of the centre of monomer A or B to this point on the microtubule.

- **Unbinding** Once bound (potential between MT and A or B is turned on) the monomer can also drop off through one of several different processes
  - **Dropping off thermally** There is a random probability p_{unbind} that at every timestep that the monomer A or B will drop off from the microtubule. Which means the bond introduced by binding is switched off
  - **Streching of bond/excessive force** If the force between A or B and the MT is above a certain value (given by a distance) the monomer A or B will drop off, defined as the bond being switched off
  - **End dropping** If the binding location of the monomer A or B is near the end of the microtubule, the monomer A or B will drop off with probability 1 (modifiable later)

Active Forces

Finally, in addition to all of the dynamics defined above, we include the effect of active driving from the bound A or B monomers to the microtubule. A monomer A or B, once bound, exerts a force on the microtubule.. The direction is defined as the vector joining monomers on the microtubule closest to the point at which the monomer A or B is bound, this force is equally applied to every monomer of the microtubule rather than just locally, under the assumption that the propagation of the forces is instant. Additionally, this force is exerted in the direction defined by polarity$_a$ and polarity$_b$, which moves towards the head or the tail of the microtubule depending on whether these values are 1 or -1. The magnitude of the force exerted is then given by:

$$|F| = \frac{1}{2} v0_a \tag{6}$$

Commensurate with this, the position at which the monomer A or B is bound to the microtuble is changed by an increment of $v0_a/gamma$, which has the effect of dragging monomer A or B along the microtubule.

Additionally, for each monomer attached to a microtubule. Additionally, the effect of monomers driving the microtubule is not purely additive, in that the total driving force is additive. The total new force F_i^{new} is updated by normalizing it such that:

$$M^2 = \sum_{\text{bound monomers}} F_i \tag{7}$$

$$f = \frac{M^2}{m_s v_0^2} \coth\left(\frac{M^2}{m_s v_0^2}\right) \tag{8}$$

$$F_i^{\mathrm{new}} = F_i / f \tag{9}$$

where m_s is the maximum number of motors exerting force. In practice this is set to 1 so the total force exerted on the microtubule is independent of the number of motors on it.