Dynein Model Explanation and Theory **John Waczak**
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General Theory

Our model for dyenin consists of a system of domains treated as spheres connected by massless rigid rods. Because dynein works inside of cells, it's aqueous environment exaggerates the forces due to drag and adds an extra random force due to collisions with water molecules. This results in the following equation of motion known as the Langevin equation:

$$m\ddot{\mathbf{x}} = \mathbf{F}_{\text{interact}} - \gamma\dot{\mathbf{x}} + \mathbf{R} \tag{1}$$

In our simulation, we use Brownian dynamics which assumes that the drag great enough so that acceleration may be neglected and, therefore, equation (1) reduces to

$$\dot{\mathbf{x}} = \frac{1}{\gamma}\left(\mathbf{F}_{\text{interact}} + \mathbf{R}\right) \tag{2}$$

where $\mathbf{x}$ is the position of the Brownian particle and $\mathbf{R}$ is the random force due to water molecule collisions. γ is the drag coefficient and depends on the radius of the Brownian particle. $\mathbf{F}_{\text{interact}}$ is the force of interaction between the particles. For our purposes, this interaction is composed of two separate forces. Our massless rods are rigid and therefore there is a tension force between adjacent domains responsible for maintaining the length constraint. We also apply a Hooke's law restorative torque with a magnitude given by

$$\Gamma_i = c_i(\varphi_i - \varphi_{i,\text{eq}}) \tag{3}$$

where c_i is a constant and $\varphi_{i,\text{eq}}$ the equilibrium angle for the i^{th} domain. The forces that these torques exert move the protein towards a preferred configuration and helps generate directed motility. Given this information, we can now discuss how these forces are determined for each of the simulation's possible states.

One bound Model

The following figure shows the model in the one bound configuration.

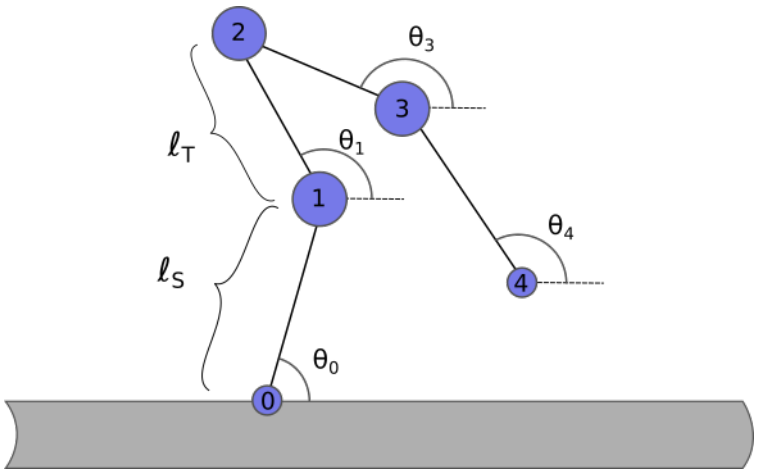

Figure 1: The dynein model in the one bound state

Here ℓ_S, ℓ_T are fixed stalk and tail lengths. We have chosen the angles $\{\theta_i\}$ as they are the most convenient and lead to a description of the position of each domain that requires only one angle and an adjacent position, that is

$$x's \quad \begin{cases} x_0 = x_{\text{bound}} \\ x_1 = x_0 + \ell_S \cos\theta_0 \\ x_2 = x_1 + \ell_T \cos\theta_1 \\ x_3 = x_2 + \ell_T \cos(\pi - \theta_3) = x_2 - \ell_T \cos\theta_3 \\ x_4 = x_3 + \ell_S \cos(\pi - \theta_4) = x_3 - \ell_S \cos\theta_4 \end{cases} \tag{4}$$

$$y's \quad \begin{cases} y_0 = 0 \\ y_1 = y_0 + \ell_S \sin\theta_0 \\ y_2 = y_1 + \ell_T \sin\theta_1 \\ y_3 = y_2 - \ell_T \sin\theta_3 \\ y_4 = y_3 - \ell_S \sin\theta_4 \end{cases} \tag{5}$$

Because equation (2) relates the forces on each domain to its velocity we need the time derivative of the above equations.

$$\dot{x}'s \quad \begin{cases} \dot{x}_0 = 0 \\ \dot{x}_1 = \dot{x}_0 - \ell_S \sin\theta_0 \dot{\theta}_0 \\ \dot{x}_2 = \dot{x}_1 - \ell_T \sin\theta_1 \dot{\theta}_1 \\ \dot{x}_3 = \dot{x}_2 + \ell_T \sin\theta_3 \dot{\theta}_3 \\ \dot{x}_4 = \dot{x}_3 + \ell_S \sin\theta_4 \dot{\theta}_4 \end{cases} \tag{6}$$

$$\dot{y}'s \quad \begin{cases} \dot{y}_0 = 0 \\ \dot{y}_1 = \dot{y}_0 + \ell_S \cos\theta_0 \dot{\theta}_0 \\ \dot{y}_2 = \dot{y}_1 + \ell_T \cos\theta_1 \dot{\theta}_1 \\ \dot{y}_3 = \dot{y}_2 - \ell_T \cos\theta_3 \dot{\theta}_3 \\ \dot{y}_4 = \dot{y}_3 - \ell_S \cos\theta_4 \dot{\theta}_4 \end{cases} \tag{7}$$