

Mechanical Description of Dynein Movement

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Dynein is a dimer protein. Each of the two subunits is composed of six or seven units, tail, and stoke. Thus it is better to treat each protein as a system of atoms. Every atom can be treated as a point mass that follows mechanics in the classical treatment. In this viewpoint, we can use classical mechanics of the descriptions for dynein movement. In the present research note, moment of globular structure of dynein amino acid sequence is given since those parts are adaptive for moment description. The moments are calculated from a coordinate (a, b, c) which is usually gravity centre of a class of point masses and every point mass exists on $\mathbf{r}_i = (x_i, y_i, z_i)$. Each point mass satisfies the classical Newton equation, namely $m_i d^2 \mathbf{r}_i / dt^2 = \sum_j \mathbf{f}_{ij}(\mathbf{r}_i)$ where $\mathbf{f}_{ij}(\mathbf{r}_i)$ is the force acting on i-th point mass from j-th point mass. We sum over all j-th point masses. Actually Newtonian equation of motion is independent of the coordinate (a, b, c) which is moved with a constant velocity. This is said to be the origin of the framework is moving constant velocity. The origin movement is correspond to dynein which is walking on microtubule rail. The constant velocity is our assumption. Thus we can apply classical Newton equation in simple manner.

The moments of point mass system are described in the following equation that is better to use a matrix form.

$$\mathbf{I} = \begin{pmatrix} I_{xx} & I_{xy} & I_{xz} \\ I_{yx} & I_{yy} & I_{yz} \\ I_{zx} & I_{zy} & I_{zz} \end{pmatrix}$$

In the above notation we use the respective momonets are followed below definition,

$$\begin{aligned} I_{xx} &= \sum_i m_i (x_i - a)(x_i - a), \quad I_{xy} = \sum_i m_i (x_i - a)(y_i - b) = I_{yx}, \quad I_{xz} = \sum_i m_i x_i (x_i - a)(z_i - c) = I_{zx}, \\ I_{yy} &= \sum_i m_i (y_i - b)(y_i - b), \quad I_{yz} = \sum_i m_i (y_i - b)(z_i - c) = I_{zy}, \quad I_{zz} = \sum_i m_i (z_i - c)(z_i - c). \end{aligned}$$

The second derivatives with respect to time are as follows:

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$$\frac{d^2 \mathbf{I}}{dt^2} = \begin{pmatrix} \frac{d^2 I_{xx}}{dt^2} & \frac{d^2 I_{xy}}{dt^2} & \frac{d^2 I_{xz}}{dt^2} \\ \frac{d^2 I_{yx}}{dt^2} & \frac{d^2 I_{yy}}{dt^2} & \frac{d^2 I_{yz}}{dt^2} \\ \frac{d^2 I_{zx}}{dt^2} & \frac{d^2 I_{zy}}{dt^2} & \frac{d^2 I_{zz}}{dt^2} \end{pmatrix}$$

The detail forms of the second derivatives in the above equation are given as follows:

$$\begin{aligned} d^2 I_{xx}/dt^2 &= 2\Sigma_i(1/m_i)(p_x^i - a)(p_x^i - a) + 2\Sigma_i(x_i - a)dp_x^i/dt = 2\Sigma_i(1/m_i)(p_x^i - a)(p_x^i - a) \\ &\quad + 2\Sigma_i(x_i - a)\Sigma_j f_{ij}(x_i) \\ d^2 I_{xy}/dt^2 &= \Sigma_i(1/m_i)(p_y^i - b)(p_x^i - a) + \Sigma_i(y_i - b)dp_x^i/dt + \Sigma_i(1/m_i)(p_x^i - a)(p_y^i - b) + \Sigma_i(x_i - a)dp_y^i/dt \\ &= \Sigma_i(1/m_i)(p_y^i - b)(p_x^i - a) + \Sigma_i(y_i - b)\Sigma_j f_{ij}(x_i) + \Sigma_i(1/m_i)(p_x^i - a)(p_y^i - b) + \Sigma_i(x_i - a)\Sigma_j f_{ij}(y_i) \\ &= d^2 I_{yx}/dt^2 \\ d^2 I_{xz}/dt^2 &= \Sigma_i(1/m_i)(p_z^i - c)(p_x^i - a) + \Sigma_i(z_i - c)dp_x^i/dt + \Sigma_i(1/m_i)(p_x^i - a)(p_z^i - c) + \Sigma_i(x_i - a)dp_z^i/dt \\ &= \Sigma_i(1/m_i)(p_z^i - c)(p_x^i - a) + \Sigma_i(z_i - c)\Sigma_j f_{ij}(x_i) + \Sigma_i(1/m_i)(p_x^i - a)(p_z^i - c) + \Sigma_i(x_i - a)\Sigma_j f_{ij}(z_i) \\ &= d^2 I_{zx}/dt^2 \\ d^2 I_{yy}/dt^2 &= 2\Sigma_i(1/m_i)(p_y^i - b)(p_y^i - b) + 2\Sigma_i(y_i - b)dp_y^i/dt \\ &= 2\Sigma_i(1/m_i)(p_y^i - b)(p_y^i - b) + 2\Sigma_i(y_i - a)\Sigma_j f_{ij}(y_i) \\ d^2 I_{yz}/dt^2 &= \Sigma_i(1/m_i)(p_z^i - c)(p_y^i - b) + \Sigma_i(z_i - c)dp_y^i/dt + \Sigma_i(1/m_i)(p_y^i - b)(p_z^i - c) + \Sigma_i(y_i - b)dp_z^i/dt \\ &= \Sigma_i(1/m_i)(p_z^i - c)(p_y^i - b) + \Sigma_i(z_i - c)\Sigma_j f_{ij}(y_i) + \Sigma_i(1/m_i)(p_y^i - b)(p_z^i - c) + \Sigma_i(y_i - b)\Sigma_j f_{ij}(z_i) \\ &= d^2 I_{zy}/dt^2 \\ d^2 I_{zz}/dt^2 &= 2\Sigma_i(1/m_i)(p_z^i - c)(p_z^i - c) + 2\Sigma_i(z_i - c)dp_z^i/dt = 2\Sigma_i(1/m_i)(p_z^i - c)(p_z^i - c) + 2\Sigma_i(z_i - c)\Sigma_j f_{ij}(z_i) \end{aligned}$$

In the above descriptions, momentums p_x^i , p_y^i , and p_z^i are defined in the following manner:

$$p_x^i = m_i dx_i/dt, \quad p_y^i = m_i dy_i/dt, \quad p_z^i = m_i dz_i/dt.$$

As seen in the above equations, the coordinate (a, b, c) is time independent, while the origin of Newtonian frame is moving $\mathbf{R}_0 = (x_0, y_0, z_0)$ with constant velocity, namely $\mathbf{R}_0 \cdot t = (x_0, y_0, z_0) \cdot t$. As already said, the movement of origin of frame is independent to the movement by classical Newton mechanics.

In this talk, we present that actual calculation of moment is important to consider dynein movement. The eigenvalue equation is the third order one because we only consider 3 by 3 matrix for three-dimensional movement of dynein. The third order equation is given by

$$\lambda^3 - \text{Tr}(\mathbf{I}) \times \lambda^2 + C_1 \times \lambda - \det(\mathbf{I}) = 0,$$

Here we define $\text{Tr}(\mathbf{I})$, C_1 , and $\det(\mathbf{I})$ as follows.

$$\text{Tr}(\mathbf{I}) = I_{xx} + I_{yy} + I_{zz},$$

$$C_1 = I_{xy}I_{yx} + I_{xz}I_{zx} + I_{yz}I_{zy} - I_{xx}I_{yy} - I_{yy}I_{zz} - I_{zz}I_{xx}$$

$$\det(\mathbf{I}) = I_{xx}I_{yy}I_{zz} + I_{xy}I_{yz}I_{zx} + I_{xz}I_{zy}I_{yx} - I_{xz}I_{yy}I_{zx} - I_{yz}I_{zy}I_{xx} - I_{xy}I_{yx}I_{zz}$$

In the figures below, an example for atom sequence from 7,994 to 10,639 that is to say a little bit four sided pyramid, but we treated with a globular unit as shown in Fig. 1. In Fig. 2, the moment calculation for that atom sequence is shown. Total atoms are 20,748.

It is said that the dynein moved on microtubule rail so that total picture of chainA is important

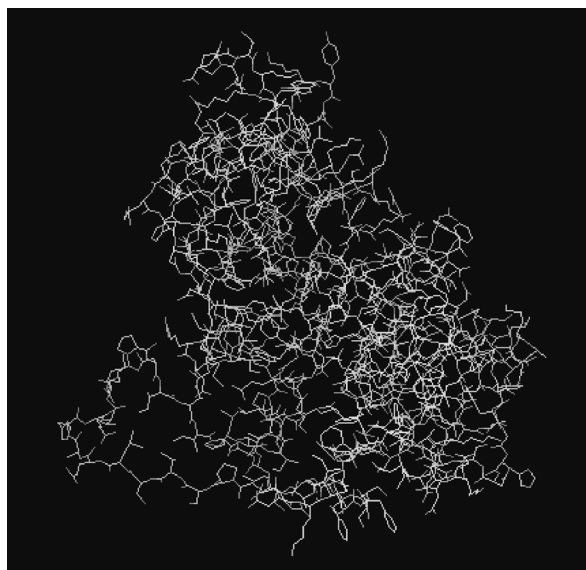


Fig. 1 RasMol figure for an atom sequence from 7994 to 10639

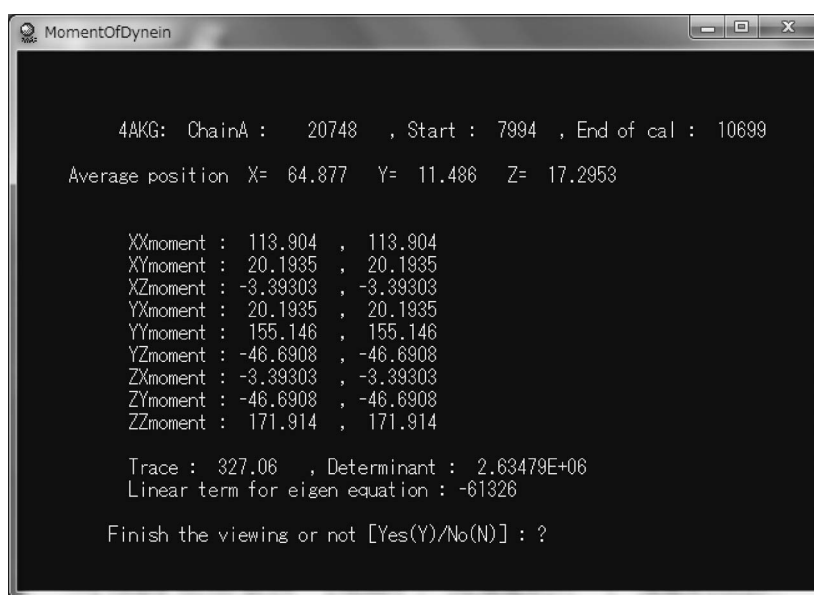


Fig. 2 Moment calculation result for atom sequence from 7994 to 10699. (a, b, c) is corresponding to average position. The values of $\text{Tr}(\mathbf{I})$, C_1 , $\det(\mathbf{I})$ are also depicted in the figure.

what shape it has. The figure of dynein chain A is shown in Fig. 3. The moment of dynein chainA is also depicted and shown in Fig. 4.

We presented equations of moments are how combine to Newtonain equation of motion. The dynein is a system of point masses and say to be globular protein in the viwpoint of protein struc-

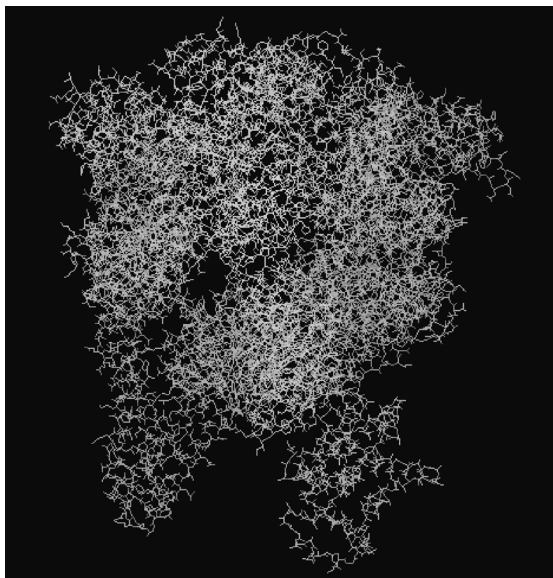


Fig. 3 RasMol figure for 4AKG chainA.

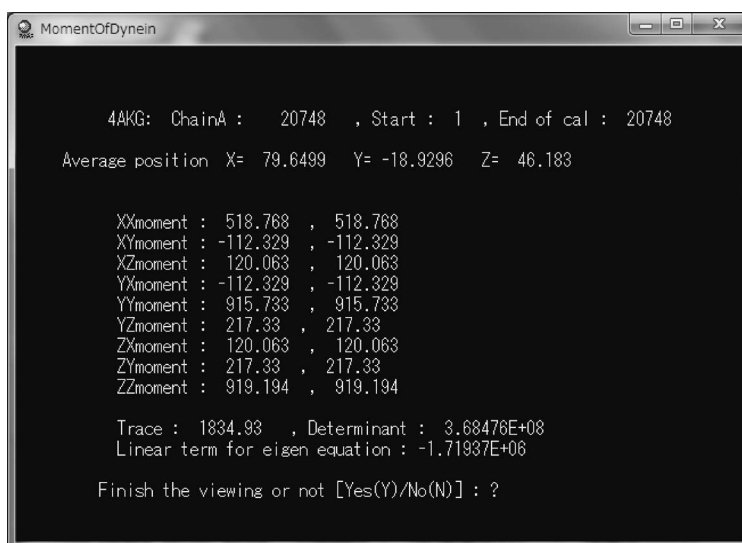


Fig. 4 Moments of whole atoms of chainA. Actually some part of sequence is missing.

tures. The moment description is effective to consider the dynein movement. But we could not discuss a dynein movement is walking on microtubules, and not calculate speed of dynein. We only use of PDB data to carry out in the calculation of moment. Thus we could not determine the frame of moving dynein from the PDB data. The consideration of dynein movement is next stage of our approach, but it requires another viewpoint of dynein movement of microtubules.