

$$\begin{aligned}
F &= F_{bulk} = \int (f_{splay} + f_{twist} + f_{bend}) d^3 \vec{r} \\
&= \int \frac{1}{2} (K_1 (\nabla \cdot \vec{n})^2 + K_2 (\vec{n} \cdot (\nabla \times \vec{n}))^2 + K_3 (\vec{n} \times (\nabla \times \vec{n}))^2) d^3 \vec{r}
\end{aligned}$$

$$U_{GB}(\hat{u}_i, \hat{u}_j, \vec{r}_{ij}) = 4\epsilon(\hat{u}_i, \hat{u}_j, \vec{r}_{ij}) \left(\frac{1}{R^{12}(\hat{u}_i, \hat{u}_j, \vec{r}_{ij})} - \frac{1}{R^6(\hat{u}_i, \hat{u}_j, \vec{r}_{ij})} \right)$$

$$U_{sphere}(\hat{u}, \vec{r}) = 4\epsilon_0 \left(\frac{1}{R^{18}(\hat{u}, \vec{r})} \right) - W \frac{(\hat{r} \cdot \hat{u})^6}{r^6}$$

$$Q = \frac{1}{N} \sum_i^N (u_{\alpha}^{(i)} u_{\beta}^{(i)} - \frac{1}{3} \delta_{\alpha\beta}) = \frac{1}{N} \sum_i^N \begin{bmatrix} u_x^{(i)} u_x^{(i)} - \frac{1}{3} & u_x^{(i)} u_y^{(i)} & u_x^{(i)} u_z^{(i)} \\ u_y^{(i)} u_x^{(i)} & u_y^{(i)} u_y^{(i)} - \frac{1}{3} & u_y^{(i)} u_z^{(i)} \\ u_z^{(i)} u_x^{(i)} & u_z^{(i)} u_y^{(i)} & u_z^{(i)} u_z^{(i)} - \frac{1}{3} \end{bmatrix}$$

$$Q_{diag} = \begin{bmatrix} -\frac{1}{3}S-\eta & 0 & 0 \\ 0 & -\frac{1}{3}S+\eta & 0 \\ 0 & 0 & \frac{2}{3}S \end{bmatrix}$$

$$2\pi s = \oint d\theta$$

$$v_i(t+\frac{\Delta t}{2})=v_i(t)+a_i(t)\frac{\Delta t}{2}$$

$$x_i(t+\Delta t) = x_i(t) + v_i(t+\frac{\Delta t}{2})\Delta t$$

$$v_i(t+\Delta t) = v_i(t+\frac{\Delta t}{2}) + a_i(t+\frac{\Delta t}{2})\frac{\Delta t}{2}$$

$$e_i(t+\Delta t) = e_i(t) + u_i(t+\frac{\Delta t}{2})\Delta t + \lambda e_i(t)\Delta t$$

$$u_i(t+\Delta t) = u_i(t+\frac{\Delta t}{2}) + \alpha_i(t+\Delta t)\frac{\Delta t}{2} + \tilde{\lambda} e_i(t+\Delta t)\frac{\Delta t}{2}$$