Calculating anisotropic elastic terms

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1 Discretization of Q-tensor equation

To begin, we need to discretize the Q-tensor equation in time, and then in space. The equation without hydrodynamics reads:

$$\frac{\partial Q}{\partial t} = H \tag{1}$$

with H given by:

$$\begin{aligned} H = 2\alpha Q - n k_B T \Lambda + 2 L_1 \nabla^2 Q \\ + L_2 \left(\nabla \left(\nabla \cdot Q \right) + \left[\nabla \left(\nabla \cdot Q \right) \right]^T - \tfrac{2}{3} \left(\nabla \cdot \left(\nabla \cdot Q \right) \right) I \right) \\ + L_3 \left(2 \nabla \cdot \left(Q \cdot \nabla Q \right) - \left(\nabla Q \right) : \left(\nabla Q \right)^T + \tfrac{1}{3} \left| \nabla Q \right|^2 I \right) \end{aligned} \tag{2}$$

To discretize in time, we use a semi-implicit method:

$$\frac{Q - Q_0}{\delta t} = 2\alpha Q_0 - n k_B T \Lambda(Q) + L_1 E^{(1)}(Q, \nabla Q) + L_2 E^{(2)}(Q, \nabla Q) + L_3 E^{(3)}(Q, \nabla Q) \tag{3}$$

where we have defined each of the elastic terms E_i as functions of Q and its gradients. To discretize in space, we define a residual which we would like to find the zeros of:

$$\begin{aligned} \mathcal{R}(Q) = \left< \phi, Q \right> - (1 + 2\alpha \delta t) \left< \phi, Q_0 \right> - \delta t \big(n k_B T \left< \phi, \Lambda(Q) \right> + L_1 \left< \phi, E^{(1)}(Q, \nabla Q) \right> \\ + L_2 \left< \phi, E^{(2)}(Q, \nabla Q) \right> + L_3 \left< \phi, E^{(3)}(Q, \nabla Q) \right> \big) \end{aligned} \tag{4}$$

We may make this a vector by specifying the test functions which we would like to integrate against:

$$\phi_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \phi_2 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \phi_3 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \phi_4 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \phi_5 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \tag{5}$$

so that:

$$\begin{aligned} \mathcal{R}_i(Q) = \left< \phi_i, Q \right> - (1 + 2\alpha \delta t) \left< \phi_i, Q_0 \right> - \delta t \big(n k_B T \left< \phi_i, \Lambda(Q) \right> + L_1 \mathcal{E}_i^{(1)}(Q, \nabla Q) \\ + L_2 \mathcal{E}_i^{(2)}(Q, \nabla Q) + L_3 \mathcal{E}_i^{(3)}(Q, \nabla Q) \big) \end{aligned} \tag{6}$$

where we have that:

$$\begin{aligned} \mathcal{E}_i^{(1)} &= \left< \phi_i, E^{(1)} \right> \\ &= 2 \left< \phi_i, \frac{\partial Q}{\partial \mathbf{n}} \right>_{\partial \Omega} - 2 \left< \nabla \phi_i, \nabla Q \right> \end{aligned} \tag{7}$$

$$
\begin{aligned}
\mathcal{E}_i^{(2)} &= \left\langle \phi_i, E^{(2)} \right\rangle \\
&= 2 \left\langle \mathbf{n} \cdot \phi_i, \nabla \cdot Q \right\rangle_{\partial\Omega} - 2 \left\langle \nabla \cdot \phi_i, \nabla \cdot Q \right\rangle \\
&\qquad + \tfrac{2}{3} \left\langle \nabla \mathrm{tr}(\phi_i), \nabla \cdot Q \right\rangle - \tfrac{2}{3} \left\langle \mathrm{tr}(\phi_i) \mathbf{n}, (\nabla \cdot Q) \right\rangle
\end{aligned}
\tag{8}
$$

$$
\begin{aligned}
\mathcal{E}_i^{(3)} &= \left\langle \phi_i, E^{(3)} \right\rangle \\
&= 2 \left\langle \mathbf{n} \otimes \phi_i, Q \cdot \nabla Q \right\rangle_{\partial\Omega} - \left\langle \nabla \phi_i, Q \cdot \nabla Q \right\rangle \\
&\qquad - \left\langle \phi_i, (\nabla Q) : (\nabla Q)^T \right\rangle + \tfrac{1}{3} \left\langle \mathrm{tr}(\phi_i), \left| \nabla Q \right|^2 \right\rangle
\end{aligned}
\tag{9}
$$

Further, we may write Q in terms of the basis functions:

$$
Q = \sum_j Q_k \phi_k \tag{10}
$$

Then we may differentiate each term with respect to Q_j to find the corresponding Jacobian of the residual:

$$
\begin{aligned}
\mathcal{R}'_{ij}(Q) = \left\langle \phi_i, \phi_j \right\rangle - (1 + 2\alpha\delta t) \left\langle \phi_i, Q_0 \right\rangle - \delta t \Big(n k_B T \left\langle \phi_i, \frac{\partial \Lambda}{\partial Q_j} \right\rangle + L_1 \left\langle \phi_i, E_1(Q, \nabla Q) \right\rangle \\
+ L_2 \left\langle \phi_i, E_2(Q, \nabla Q) \right\rangle + L_3 \left\langle \phi_i, E_3(Q, \nabla Q) \right\rangle \Big)
\end{aligned}
\tag{11}
$$