Minimum energy configurations

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1 Relevant equation and weak form

It's unclear to me whether the simulations are running for long enough to reach a minimum energy configuration. To deal with this, I'm writing a Newton-Rhapson method solver which, presumably, will run much faster. To this end, the equilibrium configuration is one in which $\partial_t Q = 0$. Then the equilibrium Q-tensor is the one that fulfills the following equation:

$$\begin{aligned} 0 &= 2\alpha Q - nk_B T\Lambda + 2L_1 \nabla^2 Q \\ &\quad + L_2 \left(\nabla \left(\nabla \cdot Q \right) + \left[\nabla \left(\nabla \cdot Q \right) \right]^T - \tfrac{2}{3} \left(\nabla \cdot \left(\nabla \cdot Q \right) \right) I \right) \\ &\quad + L_3 \left(2\nabla \cdot \left(Q \cdot \nabla Q \right) - \left(\nabla Q \right) : \left(\nabla Q \right)^T + \tfrac{1}{3} \left| \nabla Q \right|^2 I \right) \end{aligned} \tag{1}$$

Note that this is the same as our discrete time evolution equation, except taking $\delta t \to \infty$. Hence, we may take the weak-form residual and Jacobian from our previous calculations, but just take $\delta t \to \infty$ and we will be left with the corresponding equations to solve for a given Newton-Rhapson iteration to find the equilibrium configuration. The weak-form residual is then:

$$\mathcal{R}_i(Q) = \alpha \left\langle \Phi_i, Q \right\rangle - \left\langle \Phi_i, \Lambda(Q) \right\rangle + \mathcal{E}_i^{(1)}(Q, \nabla Q) + L_2 \mathcal{E}_i^{(2)}(Q, \nabla Q) + L_3 \mathcal{E}_i^{(3)}(Q, \nabla Q) \tag{2}$$

and the corresponding Jacobian is:

$$\mathcal{R}'_{ij}(Q) = \alpha \left\langle \Phi_i, \Phi_j \right\rangle - \left\langle \Phi_i, \frac{\partial \Lambda}{\partial Q_j} \right\rangle + \frac{\mathcal{E}_i^{(1)}}{\partial Q_j} + L_2 \frac{\mathcal{E}_i^{(2)}}{\partial Q_j} + L_3 \frac{\mathcal{E}_i^{(3)}}{\partial Q_j} \tag{3}$$

Given this, Newton's method reads:

$$\mathcal{R}'_{ij}(Q) \delta Q_j = -\mathcal{R}_i(Q) \tag{4}$$

with each iteration given by:

$$Q^n = Q^{n-1} + \alpha \delta Q \tag{5}$$