Assemble system code generation

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1 Equation of motion for Q-tensor

See `maier-saupe-weak-form.pdf` file. The result is:

$$\begin{aligned}\partial_t Q_{ij} = \kappa Q_{ij} - \Lambda_{ij} - \frac{L_3}{2} \left(\partial_i Q_{kl}\right) \left(\partial_j Q_{kl}\right) \\ + \partial_k \partial_k Q_{ij} + \frac{L_2}{2} \left[\partial_k \partial_j Q_{ki} + \partial_k \partial_i Q_{kj} - \tfrac{2}{3} \partial_k \partial_l Q_{kl} \delta_{ij}\right] \\ + \frac{L_3}{2} \left[2 \partial_k \left(Q_{kl} \left(\partial_l Q_{ij}\right)\right) + \tfrac{1}{3} \left(\partial_k Q_{lm}\right) \left(\partial_k Q_{lm}\right) \delta_{ij}\right]\end{aligned} \tag{1}$$

2 Weak form of right-hand side

Given a traceless, symmetric test function Φ, we may take the inner product with the right-hand side of eq. (1) to get:

$$\begin{aligned}T(Q, \nabla Q) = \kappa \left\langle \Phi_{ij}, Q_{ij} \right\rangle - \left\langle \Phi_{ij}, \Lambda_{ij} \right\rangle - \frac{L_3}{2} \left\langle \Phi_{ij}, \left(\partial_i Q_{kl}\right) \left(\partial_j Q_{kl}\right) \right\rangle \\ - \left\langle \partial_k \Phi_{ij}, \partial_k Q_{ij} \right\rangle - L_2 \left\langle \partial_k \Phi_{ij}, \partial_j Q_{ki} \right\rangle - L_3 \left\langle \partial_k \Phi_{ij}, Q_{kl} \partial_l Q_{ij} \right\rangle\end{aligned} \tag{2}$$

where we have used the fact that Φ is traceless and symmetric to make the terms proportional to δ_{ij} go to zero (this just sums over the diagonal of Φ which gives zero), and have combined terms which were previously included to make sure it stayed symmetric (since Φ is symmetric, that's enforced by the inner product).

3 Weak form of Jacobian

To get the Jacobian, we take the Gateaux derivative of T:

$$\begin{aligned}dT(Q, \nabla Q)\, \delta Q = &\left. \frac{d}{d\tau} T(Q + \tau\, \delta Q, \nabla Q + \tau \nabla \delta \tau) \right|_{\tau = 0} \\ &= \kappa \left\langle \Phi_{ij}, \delta Q_{ij} \right\rangle - \left\langle \Phi_{ij}, d\Lambda_{klij} \delta Q_{ij} \right\rangle \\ &\quad - \frac{L_3}{2} \left\langle \Phi_{ij}, \left(\partial_i Q_{kl}\right) \left(\partial_j \delta Q_{kl}\right) + \left(\partial_i \delta Q_{kl}\right) \left(\partial_j Q_{kl}\right) \right\rangle \\ &\quad - \left\langle \partial_k \Phi_{ij}, \partial_k \delta Q_{ij} \right\rangle - L_2 \left\langle \partial_k \Phi_{ij}, \partial_j \delta Q_{ki} \right\rangle \\ &\quad - L_3 \left\langle \partial_k \Phi_{ij}, \delta Q_{kl}\, \partial_l Q_{ij} + Q_{kl}\, \partial_l \delta Q_{ij} \right\rangle\end{aligned} \tag{3}$$

One must take special care with the singular potential:

$$\begin{aligned} \frac{\partial}{\partial \tau} \Lambda_{ij}(Q + \tau \delta Q) \bigg|_{\tau = 0} &= \frac{\partial}{\partial \tau} \left[\Lambda_{ij}(Q) + \tau \frac{\partial \Lambda_{ij}}{\partial Q_{kl}} \, \delta Q_{kl} + \mathcal{O}(\tau^2) \right]_{\tau = 0} \\ &= \frac{\partial \Lambda_{ij}}{\partial Q_{kl}} \, \delta Q_{kl} \end{aligned} \tag{4}$$

So then the Jacobian of the singular potential is given by $d\Lambda_{ijkl} = \partial \Lambda_{ij} / \partial Q_{kl}$.