Debugging time evolution

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1 Checking periodically perturbed free energy

To check that the configuration force matches with the energy, we check the energy for a uniform configuration first, and then for a small perturbation. The latter check gives an estimate for the configuration force by the functional Taylor series expansion:

$$F(Q + \delta Q) = F(Q) + \int_\Omega \left(\frac{\delta F}{\delta Q}\bigg|_Q : \delta Q \right) dV + \mathcal{O}\left(|\delta Q|^2 \right) \tag{1}$$

with

$$\frac{\delta F}{\delta Q} = \frac{\partial f}{\partial Q} - \nabla \cdot \frac{\partial f}{\partial \left(\nabla Q \right)} \tag{2}$$

Since this holds for an arbitrary functional F, and also for an arbitrary (small) perturbation δQ, it's probably true that:

$$f(Q + \delta Q) = f(Q) + \left(\frac{\partial f}{\partial Q} - \nabla \cdot \frac{\partial f}{\partial (\nabla Q)} \right) : \delta Q + \mathcal{O}\left(|\delta Q|^2 \right) \tag{3}$$

for each component of the free energy f. For the example we test, we take Q to be:

$$Q = S_0 \begin{bmatrix} \frac23 & 0 & 0 \\ 0 & -\frac13 & 0 \\ 0 & 0 & -\frac13 \end{bmatrix} \tag{4}$$

with

$$\delta Q = S_0 \begin{bmatrix} 0 & \epsilon \sin kx & 0 \\ \epsilon \sin kx & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{5}$$

This corresponds (to first order) to a perturbation of the director so that the total configuration $(Q + \delta Q)$ is a uniform-S configuration with director $\mathbf{n} = (1, \epsilon \sin kx, 0)$.

Here, the nondimensional free energy is given by:

$$F = \int_\Omega \left(-\tfrac12 \alpha Q : Q + \left(\log 4\pi - \log Z + \Lambda : \left(Q + \tfrac13 I \right) \right) + \tfrac12 \left| \nabla Q \right|^2 \right) dV \tag{6}$$

Then we can calculate $F(Q)$ partially analytically and partially numerically. Of course the elastic part is zero, and we calculate:

$$-\tfrac12 \alpha Q : Q = -S_0^2 \frac{\alpha}{3} = -1.2153600266666669 \tag{7}$$

with $S_0 = 0.6751$ and $\alpha = 8.0$. Further, we can calculate numerically (see `calc_lambda` program with `generate_periodic_Q_tensors.py`) Λ and Z for $S_0 = 0.6751$:

$$\begin{aligned} Z &= 3.87017170996747 \\ \Lambda &= \begin{bmatrix} 3.6005952163635766 & 0 & 0 \\ 0 & -1.8002976081817883 & 0 \\ 0 & 0 & -1.8002976081817883 \end{bmatrix} \end{aligned} \tag{8}$$

Then we may calculate F by multiplying this energy density by the size of the domain. The uniform configuration check is then just to compare that number with the energy output from the simulation for a uniform configuration with the same S_0 and α values and domain size. Calculating the energy density from the mean-field interaction gives:

$$f_{\text{entropy}} = 3.60848720197831 \tag{9}$$

Running the simulation and calculating the free energy over the domain gives:

$$F_{\text{mean field}} = -11.99497833 \tag{10}$$

and calculating out the energy density from the entropy term gives:

$$F_{\text{entropy}} = 35.61419603 \tag{11}$$

Comparing these values to the energy density multiplied by $(3.1415926 \times 3.1415926)$ (the domain size) we get similar results.

We may also consider a configuration with a different S_0-value, just to be sure. Running a similar calculation with $S_0 = 0.5$, we get the following values for Λ and Z:

$$\begin{aligned} Z &= 1.8088523960817302 \\ \Lambda &= \begin{bmatrix} 2.323990879382531 & 0 & 0 \\ 0 & -1.1619954396912653 & 0 \\ 0 & 0 & 0 \end{bmatrix} \end{aligned} \tag{12}$$

Then the entropy and mean field part of the free energy density is given by:

$$\begin{aligned} f_{\text{entropy}} &= 3.100327077782174 \\ f_{\text{mean field}} &= -\frac{2}{3} \end{aligned} \tag{13}$$

Both of these corresopnd with the energy densities written to the vtu file.

The configuration force, which is exactly the functional derivative of the free energy, is given by:

$$\frac{\delta F}{\delta Q} = -\alpha Q + \Lambda - \nabla^2 Q \tag{14}$$

We need to evaluate this with the unperturbed Q-tensor – since this is just a uniform configuration, the elastic term will be zero. However, if we explicitly calculate it we find that:

$$\left.\frac{\delta F}{\delta Q}\right|_Q : \delta Q = 0 \tag{15}$$

Hence, we actually can't get any information out of this particular perturbation.

2 S-value perturbation

To actually test this, we need to take:

$$\delta Q = \epsilon \sin kx Q \tag{16}$$

Taking $k = 1$ and $\epsilon = 0.1$, we may explicitly calculate (using values previously stated):

$$\left.\frac{\delta F_{\text{mean field}}}{\delta Q}\right|_Q : \delta Q = -\tfrac{2}{3} S_0 \alpha \epsilon \sin kx = (-0.36005333333333334) \sin kx \tag{17}$$

and

$$\left.\frac{\delta F_{\text{entropy}}}{\delta Q}\right|_Q : \delta Q = \epsilon \sin kx \left(\tfrac{2}{3}\Lambda_1 - \tfrac{1}{3}\Lambda_4 + \tfrac{1}{3}(\Lambda_1 + \Lambda_4)\right) = (0.3600595216363576) \sin kx \tag{18}$$

3 Landau-de Gennes time evolution for periodically-perturbed S-value

To check the general scheme, we employ a Landau-de Gennes field theory with elastic isotropy. With this, the time evolution is governed by:

$$\frac{\partial Q}{\partial t} = -\left(AQ + B(Q \cdot Q) + C(Q : Q)Q\right) + \nabla^2 Q \tag{19}$$

First we consider a configuration with director pointing completely in the x-direction so that $\mathbf{n} = (1, 0, 0)$ and an S-value dependent on time and the x-coordinate. By symmetry, S will not depend on y or z supposing that the initial condition is only a function of x. Then we get:

$$Q(x,t) = S(x,t)\left(\mathbf{n} \otimes \mathbf{n} - \tfrac{1}{3} I\right) = S(x,t) \begin{bmatrix} \frac{2}{3} & 0 & 0 \\ 0 & -\frac{1}{3} & 0 \\ 0 & 0 & -\frac{1}{3} \end{bmatrix} \tag{20}$$

Plugging into the Landau-de Gennes time evolution equation gives:

$$3\frac{\partial S(x,t)}{\partial t} = -3AS(x,t) + BS^2(x,t) - CS^3(x,t) + 3\frac{\partial^2 S(x,t)}{\partial x^2} \tag{21}$$

Supposing a periodic initial condition:

$$S(x,0) = A_0 \sin kx \tag{22}$$

we take as an ansatz that:

$$S(x,t) = \sum_n A_n(t) \sin nkx \tag{23}$$

So that the time evolution equation becomes:

$$
\begin{aligned}
3\sum_n \sin(nkx)\frac{dA_n(t)}{dt} = & -3A\sum_n A_n(t)\sin(nkx) \\
& + B\sum_{m,n} A_m(t)A_n(t)\sin(nkx)\sin(mkx) \\
& - C\sum_{l,m,n} A_l(t)A_m(t)A_n(t)\sin(lkx)\sin(mkx)\sin(nkx) \\
& - 3\sum_n A_n(t)n^2k^2\sin(nkx) \\
= & -3A\sum_n A_n(t)\sin(nkx) \\
& + B\sum_{m,n} \tfrac{1}{2}A_m(t)A_n(t)\Big[\cos((n-m)kx) - \cos((n+m)kx)\Big] \\
& - C\sum_{l,m,n} \tfrac{1}{4}A_l(t)A_m(t)A_n(t)\Big[\sin((l+n-m)kx) + \sin((l-n+m)kx) \\
& - \sin((l+n+m)kx) - \sin((l-n-m)kx)\Big] \\
& - 3\sum_n A_n(t)n^2k^2\sin(nkx)
\end{aligned}
\tag{24}
$$