Qian-Sheng hydrodynamics reduction to Stokes equation

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1 Introduction

Here we take the Qian-Sheng formulation for hydrodynamics of nematic liquid crystals, and make several approximations to reduce it to the form of a Stokes hydrodynamic equation, coupled to an equation of motion for the nematic order parameter Q. We then introduce a weak form, and outline an algorithm for solving the weak form equation.

2 Qian-Sheng formulation and reduction

3 Full theory

The Qian-Sheng formulation consists of two coupled equations: a hydrodynamic equation which is a generalization of the Navier-Stokes equation, and a generalized force-balance equation for the thermodynamics of liquid crystals. These equations are given as follows:

$$\begin{aligned} \rho \frac{dv_i}{dt} &= \partial_j \left(-p\delta_{ji} + \sigma^d_{ji} + \sigma^f_{ji} + \sigma'_{ji} \right), \\ J\ddot{Q}_{ij} &= h_{ij} + h'_{ij} - \lambda \delta_{ij} - \epsilon_{ijk}\lambda_k \end{aligned} \tag{1}$$

These, along with the incompressibility condition $\partial_i v_i = 0$ give our equations of motion. Here we take J to be negligible, and also take the time evolution of v_i to be negligible. Additionally, we assume no external fields so that σ^f, the stress due to external fields is also zero. Now, σ^d the distortional stress is purely a result of spatial variations in the nematic order parameter, given as:

$$\sigma^d_{ij} = -\frac{\partial \mathcal{F}}{\partial(\partial_j Q_{\alpha\beta})} \partial_i Q_{\alpha\beta} \tag{2}$$

while the elastic molecular field h_{ij} is also purely a function of Q and its gradients:

$$h_{ij} = -\frac{\partial \mathcal{F}}{\partial Q_{ij}} + \partial_k \frac{\partial \mathcal{F}}{\partial(\partial_k Q_{ij})} \tag{3}$$

This is just the variation of the free energy, which gives the equilibrium solutions when the traceles, symmetric part of h_{ij} is zero.

Now, the viscous contributions to the equations of motion are given by:

$$\begin{aligned} \sigma'_{\alpha\beta} = \beta_1 Q_{\alpha\beta} Q_{\mu\nu} A_{\mu\nu} + \beta_4 A_{\alpha\beta} + \beta_5 Q_{\alpha\mu} A_{\mu\beta} + \beta_6 A_{\alpha\mu} Q_{\mu\beta} \\ + \tfrac{1}{2}\mu_2 N_{\alpha\beta} - \mu_1 Q_{\alpha\mu} N_{\mu\beta} + \mu_1 Q_{\beta\mu} N_{\mu\alpha} \end{aligned} \tag{4}$$

and

$$-h'_{\alpha\beta} = \tfrac{1}{2}\mu_2 A_{\alpha\beta} + \mu_1 N_{\alpha\beta} \tag{5}$$

where $A_{\alpha\beta}$ is the symmetrization of the velocity gradient, and $N_{\alpha\beta}$ is a measure of the rotation of the director field relative to the rotation of the fluid. Both are given by:

$$A_{ij} = \tfrac{1}{2}\left(\partial_i v_j + \partial_j v_i\right) \tag{6}$$

$$N_{ij} = \frac{dQ_{ij}}{dt} + W_{ik}Q_{kj} - Q_{ik}W_{kj} \tag{7}$$

with W_{ij} the antisymmetrization of the velocity gradient:

$$W_{ij} = \tfrac{1}{2}\left(\partial_i v_j - \partial_j v_i\right) \tag{8}$$

The β's and μ's are viscosity coefficients with the relation $\beta_6 - \beta_5 = \mu_2$.

4 Simplification and reduction to Stokes

Now, given the generalized force equation, we may solve for the time evolution of the order parameter Q_{ij}. Plugging in for the generalized forces yields:

$$\begin{aligned} h_{ij} - \lambda\delta_{ij} - \epsilon_{ijk}\lambda_k &= \tfrac{1}{2}\mu_2 A_{\alpha\beta} + \mu_1 N_{\alpha\beta} \\ \implies N_{\alpha\beta} &= \frac{1}{\mu_1}\left(h_{ij} - \lambda\delta_{ij} - \epsilon_{ijk}\lambda_k\right) - \frac{1}{2}\frac{\mu_2}{\mu_1}A_{\alpha\beta} \end{aligned} \tag{9}$$

We will use this relation later, but for now we plug in for N_{ij} and solve for an equation of motion of the order parameter:

$$\frac{dQ_{ij}}{dt} = \frac{1}{\mu_1}H_{ij} + \left(Q_{ik}W_{kj} - W_{ik}Q_{kj}\right) - \frac{1}{2}\frac{\mu_2}{\mu_1}A_{\alpha\beta} \tag{10}$$

where we have defined:

$$H_{ij} = \left(h_{ij} - \lambda\delta_{ij} - \epsilon_{ijk}\lambda_k\right) \tag{11}$$

just to tidy up the equations of motion. For the fluid equation, we only consider terms linear in Q_{ij} and v_i. This gives us the following for the stress tensor:

$$\sigma'_{\alpha\beta} = \beta_4 A_{\alpha\beta} + \tfrac{1}{2}\mu_2 N_{\alpha\beta} \tag{12}$$

Using equation (9) we may plug in to obtain an explicit Q-dependence:

$$\begin{aligned} \sigma'_{\alpha\beta} &= \beta_4 A_{\alpha\beta} + \frac{1}{2}\frac{\mu_2}{\mu_1}H_{\alpha\beta} - \frac{1}{4}\frac{\mu_2^2}{\mu_1}A_{\alpha\beta} \\ &= \left(\beta_4 - \frac{1}{4}\frac{\mu_2^2}{\mu_1}\right)A_{\alpha\beta} + \frac{1}{2}\frac{\mu_2}{\mu_1}H_{\alpha\beta} \\ &= \alpha_1 A_{\alpha\beta} + \gamma_1 H_{\alpha\beta} \end{aligned} \tag{13}$$

where we have defined the constants:

$$\alpha_1 = \beta_4 - \frac{1}{4}\frac{\mu_2^2}{\mu_1} \tag{14}$$

$$\gamma_1 = \frac{1}{2}\frac{\mu_2}{\mu_1} \tag{15}$$

Here we may rewrite the Stokes equation in a way that more closely resembles the deal.II tutorial formulation. To do this, just plug in and isolate the symmetrized velocity gradient:

$$\begin{aligned} 0 &= -\partial_j p\delta_{ij} + \partial_j\sigma^d_{ji} + \alpha_1\partial_j A_{ji} + \gamma_1\partial_j H_{ji} \\ \implies -\alpha_1\partial_j A_{ji} + \partial_j p\delta_{ij} &= \partial_j\sigma^d_{ji} + \gamma_1\partial_j H_{ji} \end{aligned} \tag{16}$$

Note that the right-hand side only depends on the Q-tensor, so for the purposes of solving for flow we may just treat it as a forcing term.

5 Nondimensionalizing the Stoke's equation

The velocity field has units of length over time, and so the symmetric gradient just has units of inverse time. Pressure has units of force per area, and so the divergence of pressure has units of force per unit volume. The same is true for stress. Finally, when we non-dimensionalized the symmetric traceless variation of the free energy H_{ij} we divided by nk_BT which is something like an energy density (by number, not by volume). Hence, rewriting in terms of nondimensional quantities gives:

$$- \alpha_1 \frac{1}{\xi\tau} \nabla \cdot \overline{A} + \frac{\kappa}{\xi^3} \nabla \overline{p} = \frac{\kappa}{\xi^3} \nabla \cdot \overline{\sigma}^d + \gamma_1 \frac{nk_BT}{\xi} \nabla \cdot \overline{H} \tag{17}$$

Now, because of the specific form of the equation of motion of Q we make the following definition for the time-scale constant:

$$\tau = \frac{\mu_1}{nk_BT} \tag{18}$$

We take the length-constant ξ to be as before (see maier-saupe-weak-form document):

$$\xi = \sqrt{\frac{2L_1}{nk_BT}} \tag{19}$$

Multiplying through by ξ and dividing by nk_BT, we get the following:

$$- \frac{\alpha_1}{\mu_1} \nabla \cdot \overline{A} + \frac{\kappa}{2L_1} \nabla \overline{p} = \frac{\kappa}{2L_1} \nabla \cdot \overline{\sigma}^d + \gamma_1 \nabla \cdot \overline{H} \tag{20}$$

Finally, multiplying through by $2\mu_1/\alpha_1$, then defining the following:

$$\begin{aligned} \kappa &= \frac{L_1 \alpha_1}{\mu_1} \\ \gamma &= \frac{\gamma_1 \alpha_1}{\mu_1} \end{aligned} \tag{21}$$

we get the familiar form of Stoke's equation:

$$- 2\nabla \cdot A + \nabla p = \nabla \cdot \sigma^d + \gamma \nabla \cdot H \tag{22}$$

where we have dropped the overlines for sake of brevity.

6 Weak form of the reduced equations

6.1 Weak form of the Stokes equation

For consistency with the deal.II tutorial programs, we take u_i to be the solution fluid velocity, and v_i to be the relevant test function components. Further, we take p to be the pressure solution and q to be the corresponding test functions. We then arrange our equations of motion as follows:

$$\begin{pmatrix} \nabla \left(-p + \boldsymbol{\sigma}^d + \boldsymbol{\sigma}' \right) \\ \nabla \cdot \mathbf{u} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{23}$$

Dotting with $(\mathbf{v} \, q)$ gives the following weak form:

$$\langle \mathbf{v}, -\nabla p \rangle + \langle \mathbf{v}, \nabla \cdot \boldsymbol{\sigma}^d \rangle + \langle \mathbf{v}, \nabla \cdot \boldsymbol{\sigma}' \rangle + \langle q, \nabla \cdot \mathbf{u} \rangle = 0 \tag{24}$$

Integrating by parts gives us the following:

$$- \langle \mathbf{n} \cdot \mathbf{v}, p \rangle_{\partial\Omega} + \langle \nabla \cdot \mathbf{v}, p \rangle + \langle \mathbf{v}, \mathbf{n} \cdot \boldsymbol{\sigma}^d \rangle_{\partial\Omega} - \langle \nabla \mathbf{v}, \boldsymbol{\sigma}^d \rangle + \langle \mathbf{v}, \mathbf{n} \cdot \boldsymbol{\sigma}' \rangle_{\partial\Omega} - \langle \nabla \mathbf{v}, \boldsymbol{\sigma}' \rangle + \langle q, \nabla \cdot \mathbf{u} \rangle = 0 \tag{25}$$

Now we plug in for σ':

$$\begin{aligned} &-\langle \mathbf{n}\cdot\mathbf{v}, p\rangle_{\partial\Omega} + \langle \nabla\cdot\mathbf{v}, p\rangle + \alpha_1\langle \mathbf{v}, \mathbf{n}\cdot\varepsilon(\mathbf{u})\rangle_{\partial\Omega} - \alpha_1\langle \nabla\mathbf{v}, \varepsilon(\mathbf{u})\rangle + \langle q, \nabla\cdot\mathbf{u}\rangle \\ &\quad = -\langle \mathbf{v}, \mathbf{n}\cdot\boldsymbol{\sigma}^d\rangle_{\partial\Omega} + \langle \nabla\mathbf{v}, \boldsymbol{\sigma}^d\rangle - \gamma_1\langle \mathbf{v}, \mathbf{n}\cdot(h - \lambda I - \varepsilon\cdot\lambda)\rangle_{\partial\Omega} + \gamma_1\langle \nabla\mathbf{v}, h - \lambda I - \epsilon\cdot\boldsymbol{\lambda}\rangle \end{aligned} \tag{26}$$

where we have defined:

$$\alpha_1 = \beta_4 - \frac{1}{4}\frac{\mu_2^2}{\mu_1} \tag{27}$$

$$\gamma_1 = \frac{1}{2}\frac{\mu_2}{\mu_1} \tag{28}$$

where α_1 is a viscosity and γ_1 is related to the propensity with which the directors are rotated by vorticity in the fluid. More specifically, $\gamma_1 = -\lambda S$ where here λ is the tumbling parameter and S is the uniaxial scalar order parameter for a constant-S system (c.f. Leslie-Ericksen hydrodynamic equations). Note that all of the fluid solution variables are on the left side, while the driving terms from the Q-tensor are on the right.

6.2 Time-discretizing the order parameter equation

Now, before we find a weak form of the order-parameter equation, we must first discretize it in time. For the diffusive part, we may employ a convex-splitting scheme, since each term in the variation of the free energy happens to be convex. However, velocity is a complicated function of Q which cannot be easily proven to be convex. For u, since we cannot find an analytic form of it as a function of Q^n, during each Newton iteration we solve for u using Q from the last Newton iteration, and then plug that u into the calculation of the residual and Jacobian for Q. We hope that this converges.

The discretized time equation is then:

$$\frac{Q^n - Q^{n-1}}{\delta t} + \mathbf{u}\cdot\nabla Q^n = \frac{1}{\mu_1}\left(h - \lambda I - \epsilon\cdot\boldsymbol{\lambda}\right) + \left(Q^n W - W Q^n\right) - \gamma_1\varepsilon(\mathbf{u}) \tag{29}$$

where $\mathbf{u}$ is calculated with both Q^n and Q^{n-1} mirroring the convex splitting of the free energy variation terms.

6.3 Newton's method for order parameter equation

Now, since this is an *implicit* equation for Q^n, we will need to solve for it iteratively using a Newton-Rhapson method. Again, at each Newton iteration we solve for u using the last Newton iteration, and then use that when calculating the Jacobian and Residual. Hence, u will be a constant in all of our calculations, only being updated by solving the Stokes equation as above.

Now, the residual of Newton's method is just given by:

$$\begin{aligned} R_i(Q^n) = \frac{Q_i^n - Q_i^{n-1}}{\delta t} + \mathbf{u}\cdot\nabla Q^n - \frac{1}{\mu_1}\left(h_{r(i)c(i)} - \lambda\delta_{r(i)c(i)} - \epsilon_{r(i)c(i)k}\lambda_k\right) \\ - \left(Q_{r(i)k}^n W_{kc(i)} - W_{r(i)k} Q_{kc(i)}^n\right) + \gamma_1\varepsilon(\mathbf{u})_{r(i)c(i)} \end{aligned} \tag{30}$$

where we have introduced index notation, and the functions $r(i)$ and $c(i)$. For this, we have considered Q_i to be a vector consisting of the independent degrees of freedom of the Q-tensor, enumerated as:

$$Q_{ij} = \begin{pmatrix} Q_1 & Q_2 & Q_3 \\ Q_2 & Q_4 & Q_5 \\ Q_3 & Q_5 & -(Q_1 + Q_4) \end{pmatrix} \tag{31}$$

Note that $r(i)$ and $c(i)$ pick out the row and column of the first occurence of the ith degree of freedom. Explicitly we have:

$$r(i) = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 2 \\ 2 \end{pmatrix}, \quad c(i) = \begin{pmatrix} 1 \\ 2 \\ 3 \\ 2 \\ 3 \end{pmatrix} \tag{32}$$

Now, we wish to find the Jacobian of this residual. To do this, we need to take a functional Gateaux derivative, whose formal definition is given by:

$$dR(Q^n, \delta Q^n = \frac{d}{d\tau} R(Q^n + \tau \delta Q^n \Big|_{\tau=0} \tag{33}$$

where δQ^n is some function whose direction we are taking the derivative in. We may consider the ith component of $dR(Q^n, \delta Q^n$, and compute it term by term:

$$\frac{d}{d\tau} \left(\frac{Q_i^n + \tau \delta Q_i^n - Q_i^{n-1}}{\delta t} \right) \Bigg|_{\tau=0} = \frac{\delta Q_i^n}{\delta t} \tag{34}$$

$$\frac{d}{d\tau} \left(u_k \partial_k (Q_i^n + \tau \delta Q_i^n) \right) \Bigg|_{\tau=0} = u_k \partial_k \delta Q_i^n \tag{35}$$