An energetic variational formulation with phase field methods for interfacial dynamics of complex fluids

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Introduction

Complex fluids are mixtures in which two phases coexists. Their response to applied strain and stress is complex and hence they are non-Newtonian fluids. One phase is generally continuous and other one is dispersed. Some examples of complex fluids are milk, blood, polymer-dispersed liquid crystals and polymer blends etc. The micro-structures of complex fluids can be manipulated to get desired mechanical or optical properties like by creating the composites of immiscible fluids. The properties of these composites can be varied by varying composition and concentration of components. Studying the dynamics of complex fluids involve coupling of three length scales, molecular conformation inside each component, mesoscopic interfacial morphology and macroscopic hydrodynamics [1]. In the two-phase systems, the interfaces are complex that can move and deform. There are many ways of handling the moving interface. One way is to use moving mesh that has grid points on the interfaces. These methods break when interfaces undergo singular topological changes like breakup and coalescence. The second way is to use Eulerian grid method in which the grid remains fixed. Examples of fixed grid methods are volume-of-fluid (VOF) method and level set method. Phase field method is motivated from the level set method.

1 Phase field method

Two phase problems generally involves a complex moving free boundary. The boundary is usually modeled by a sharp interface model. This model gives a precise location of interface which moves with a normal velocity. There can be a sudden jump in the density of extensive quantities at the sharp interface. The bulk equations are solved in each phase with matching boundary condition at the interface. The sharp interface model breaks down when the interfacial thickness is of the order radius of curvature of surfaces. Second way of defining boundary is the diffusive field model which assumes that the interface has some thickness and all extensive quantities varies smoothly in the interface region. The phase field method is a diffusive interface method. It introduces additional phase field variables which varies slowly in the bulk and rapidly in the interfacial region. Interfacial region is a narrow region where two phases mix even though they are immiscible. The phase field method is similar to level set method but instead of using artificial smoothing function a physical scalar field (phase field) is used. Asymptotically, when the thickness of interface approaches zero, the phase field model corresponds to the sharp interface formulations.

2 Energy based phase field theory

The energy based formulation is done for the blend of a Newtonian viscous fluid and nematic liquid crystal with planar anchoring. For this kind of blend, there are three types of free energy (a) mixing energy at the interface, (b) Distorting energy in the bulk for the liquid crystal and (c) the anchoring energy of the liquid crystal at the surface.

2.1 Mixing energy

In the diffusive interface model, interface has finite thickness in which the immiscible fluid mixes. The regularized form of the mixing energy given by Cahn and Hilliard is given by [2]

$$f_{mix}(\phi, \nabla \phi) = f_0(\phi) + \frac{\lambda}{2} |\nabla \phi|^2, \qquad (1)$$

where λ is called the mixing energy density and ϕ is the phase field variable which is related to the concentrations of two components as

$$c_1 = \frac{1+\phi}{2}$$
 and $c_2 = \frac{1-\phi}{2}$. (2)

For the phase separation to happen the free energy function should have two minima and a maxima in between (double well potential) [3]. Figure 1 shows a simple double well potential. The simplest double well potential is given by

$$f_0(\phi) = Ac_i^2 (1 - c_i^2)^2 = \frac{A}{4} (\phi^2 - 1)^2 = \frac{\lambda}{4\epsilon^2} (\phi^2 - 1)^2,$$
(3)

where ϵ is a capillary width and it represents the thickness of the interface (see (7)). The gradient energy term, $\lambda |\nabla \phi|^2/2$ term competes with the bulk energy term f_0 to give a diffused boundary. f_{mix} represents the molecular interaction between the two phases in the interfacial region and hance can be related to the surface tension at the interface. The surface energy at the interface for the 1D case can be written using (1) as,

$$\sigma = \int_{-\infty}^{+\infty} \frac{\lambda}{2} \left(\frac{d\phi}{dx}\right)^2 + f_0(\phi) dx.$$
(4)

If we assume the diffuse interface at equilibrium then its variation is zero and thus

$$\frac{d^2\phi}{dx^2} = \frac{f_0'(\phi)}{\lambda}.$$
(5)

Integrating the above equation once and assuming that everything vanishes at the infinity, we get

$$\left(\frac{d\phi}{dx}\right)^2 = \frac{2f_0(\phi)}{\lambda}.\tag{6}$$

Substituting, $f_0(\phi)$ from (3) and setting $\phi(0) = 0$ in the above equation, we obtain

$$\phi(x) = \tanh\left(\frac{x}{\sqrt{2\epsilon}}\right).\tag{7}$$

 $\phi = 0$ can be interpreted as the mid point of the diffuse interface where concentration of both the phases are equal. Figure 2 shows the plot of ϕ with non-dimensionalized $\hat{x} = x/\epsilon$. From the Fig. , we find that the 99% of variation in ϕ happens within the thickness of 7.5 ϵ . Hence ϵ represents the scale of the thickness of interface.

Finally, we can substitute (7) in (4) to get,

$$\sigma = \int_{-\infty}^{+\infty} \frac{\lambda}{2} \frac{1}{(\sqrt{2}\epsilon)^2} \left(1 - \tanh^2\left(\frac{x}{\sqrt{2}\epsilon}\right) \right)^2 + \frac{\lambda}{4\epsilon^2} \left(\tanh^2\left(\frac{x}{\sqrt{2}\epsilon}\right) - 1 \right)^2 dx \tag{8}$$

$$= \int_{-\infty}^{+\infty} \frac{\lambda}{2\epsilon^2} \left(1 - \tanh^2\left(\frac{x}{\sqrt{2}\epsilon}\right) \right)^2 dx$$

$$= \frac{\lambda}{2\epsilon^2} \sqrt{2}\epsilon \left[\tanh\left(\frac{x}{\sqrt{2}\epsilon}\right) - \frac{1}{3} \tanh^3\left(\frac{x}{\sqrt{2}\epsilon}\right) \right]_{-\infty}^{+\infty}$$

$$= \frac{2\sqrt{2}\lambda}{3\epsilon}$$

2.2 Bulk distortion energy

Nematic liquid crystals are organic materials formed by elongated molecules like rods or ellipsoids . The long molecular axis are aligned along a common direction \mathbf{n} which is called the director. If the director is independent of the spatial coordinates then the medium is undistorted and the distortion energy is minimum. The Frank distortion energy density of a deformed NLC is given by

$$f_{Frank} = \frac{1}{2} \left\{ K_1(\nabla .\mathbf{n})^2 + K_2(\mathbf{n}.\nabla \times \mathbf{n})^2 + K_3(\mathbf{n} \times \nabla \times \mathbf{n})^2 \right\} - (K_2 + K_4)\nabla \cdot (\mathbf{n}\nabla \cdot \mathbf{n} + \mathbf{n} \times \nabla \times \mathbf{n}), \quad (9)$$

where K_1, K_2, K_3 and $(K_2 + K_4)$ are called splay, twist, bend and saddle-splay elastic constants, respectively [4]. These states of distortion are depicted in Fig. 3. The last term of the above expression contributes only on the surface due to divergence theorem. To simplify the Frank distortion energy, we will assume $K = K_1 = K_2 = K_3 = \text{and } K_4 = 0$. Substituting these in the above equation and using the following identities,

$$(\mathbf{n} \cdot \nabla \times \mathbf{n})^2 + (\mathbf{n} \times \nabla \times \mathbf{n})^2 = n_{i,j} n_{i,j} - n_{i,j} n_{j,i},$$
(10)

$$(\nabla \mathbf{n})^2 - \nabla \cdot (\mathbf{n} \nabla \cdot \mathbf{n} + \mathbf{n} \times \nabla \times \mathbf{n}) = n_{i,j} n_{j,i}, \qquad (11)$$

we obtain,

$$f_{Frank} = \frac{K}{2} n_{i,j} n_{i,j} = \frac{K}{2} \nabla \mathbf{n} : \nabla \mathbf{n}.$$
(12)

The frank theory fails at singular points (defects) where $|\mathbf{n}| = 0$. To overcome this, [5] used regularized Frank elastic energy,

$$f_{bulk} = K \left\{ \frac{1}{2} \nabla \mathbf{n} : \nabla \mathbf{n} + \frac{(|\mathbf{n}|^2 - 1)^2}{4\delta^2} \right\}.$$
(13)

The gradient of the second term $F_L(|\mathbf{n}|) = (|\mathbf{n}|^2 - 1)^2/4\delta^2$ is the penalty function

$$f_L(\mathbf{n}) = \frac{(|\mathbf{n}|^2 - 1)\mathbf{n}}{\delta^2},\tag{14}$$

which is used to approximate the constraint $|\mathbf{n}| = 1$.

2.3 Anchoring energy

The anchoring is a phenomenon of orientation of a liquid crystal by the surface in a preferred direction called anchoring direction or easy direction. The anchoring energy is a measure of energy required to deviate from the easy direction. If every direction in the plane is an easy direction then it is called planar anchoring. When the easy direction lies along the normal of a plane then it is called homeotropic anchoring. We will only consider the case of planar anchoring. The Rapini-Popoular anchoring energy for sharp-interface model is given as

$$f_{anch} = -\frac{W}{2} (\mathbf{n} \cdot \mathbf{n_0}), \tag{15}$$

where $\mathbf{n_0}$ is the surface easy direction and W is the anchoring strength. Motivated by (15), for diffuse-interface, the volumetric energy density for planar anchoring is written as

$$f_{anch} = \frac{A}{2} (\mathbf{n} \cdot \nabla \phi)^2, \tag{16}$$

Summing all the three free energy, we get the total free energy

$$f(\phi, \mathbf{n}, \nabla \phi, \nabla \mathbf{n}) = f_{mix} + \frac{1+\phi}{2} f_{bulk} + f_{anch}$$

= $\frac{\lambda}{2} \left(|\nabla \phi|^2 + \frac{1}{2\epsilon^2} (\phi^2 - 1)^2 \right) + \frac{K(1+\phi)}{2} \left(\frac{1}{2} \nabla \mathbf{n} : \nabla \mathbf{n} + \frac{(|\mathbf{n}|^2 - 1)^2}{4\delta^2} \right) + \frac{A}{2} (\mathbf{n} \cdot \nabla \phi)^2 \quad (17)$

where $(1 + \phi)/2$ is the volume fraction of the nematic liquid crystal in the bulk. The surface tension in the sharp interface limit can be obtained by making $\epsilon \to 0$.

2.4 Governing equation using variations

T In the absence of dissipative forces, the system of governing equation can be obtained by variational principles. The langrangian is given by

$$L = \int_{t_1}^{t_2} \int_{\omega} \rho\left(\frac{1}{2}|\mathbf{v}|^2 - f(\phi, \mathbf{n}, \nabla\phi, \nabla\mathbf{n})\right) d\mathbf{x} dt$$
(18)

where ω represents the domain in the current configuration at t and $\mathbf{v}(\mathbf{X}, t) = \dot{\mathbf{x}}(\mathbf{X}, t)$ is the velocity of particles. **X** is the locations of particles in the initial configuration at t = 0 and **x** is location in the current configuration at time t. Let $\mathbf{x}_{\varepsilon}(\mathbf{X}, t), \phi_{\varepsilon}(\mathbf{x}, t)$ and $\mathbf{n}_{\varepsilon}(\mathbf{x}, t)$ be defined as

$$\mathbf{x}_{\varepsilon}(\mathbf{X}, t) = \mathbf{x}(\mathbf{X}, t) + \varepsilon \boldsymbol{\psi}(\mathbf{x}, t), \tag{19}$$

$$\phi_{\varepsilon}(\mathbf{x},t) = \phi(\mathbf{x},t) + \varepsilon \chi(\mathbf{x},t), \qquad (20)$$

$$\mathbf{n}_{\varepsilon}(\mathbf{x},t) = \mathbf{n}(\mathbf{x},t) + \varepsilon \boldsymbol{\zeta}(\mathbf{x},t), \tag{21}$$

where ψ, χ and ζ are the variations of x, ϕ and n, respectively. Using (19), we can write $\mathbf{v}_{\varepsilon}(\mathbf{X}, t)$ as,

$$\mathbf{v}_{\varepsilon}(\mathbf{X},t) = \dot{\mathbf{x}}(\mathbf{X},t) + \varepsilon \dot{\boldsymbol{\psi}}(\mathbf{x},t), \qquad (22)$$

Also, by taking gradient of (19) with respect to \mathbf{x}_{ε} , we get

$$\nabla_{\varepsilon} \mathbf{x} = \mathbf{I} - \varepsilon \nabla_{\varepsilon} \boldsymbol{\psi}, \tag{23}$$

where \mathbf{I} is the identity matrix. Similarly taking gradient of (20) and using the above expression, we get

$$\begin{aligned} \nabla_{\varepsilon}\phi_{\varepsilon} &= \nabla_{\varepsilon}\phi + \varepsilon\nabla_{\varepsilon}\chi, \\ &= \{\mathbf{I} - \varepsilon\nabla_{\varepsilon}\psi\}\,\nabla\phi + \varepsilon\nabla_{\varepsilon}\chi, \\ &= \nabla\phi - \varepsilon\nabla_{\varepsilon}\psi\nabla\phi + \varepsilon\nabla_{\varepsilon}\chi. \end{aligned}$$
(24)

Similarly,

$$\nabla_{\varepsilon} \mathbf{n}_{\varepsilon} = \nabla \mathbf{n} - \nabla_{\varepsilon} \boldsymbol{\psi} \nabla \boldsymbol{n} + \varepsilon \nabla_{\varepsilon} \boldsymbol{\zeta}, \qquad (25)$$

In the absence of diffusion, ϕ and **n** is simply advected and thus

$$\phi(\mathbf{x},t) = \phi_0(\mathbf{X}) \quad \text{and} \quad \mathbf{n}(\mathbf{x},t) = \mathbf{n}_0(\mathbf{X})$$
(26)

and hence variations of ϕ and **n** are zero. Also the density $\rho(\mathbf{x}, t)$ is given as

$$\rho(\mathbf{x}, t) = \frac{\rho_0(\mathbf{X})}{J} \quad \text{where} \quad J = \det\left(\frac{d\mathbf{x}}{d\mathbf{X}}\right). \tag{27}$$

Calculating the first variation of L,

$$\frac{d}{d\varepsilon}L(\boldsymbol{v}_{\varepsilon},\phi,\boldsymbol{n},\nabla_{\varepsilon}\phi,\nabla_{\varepsilon}\boldsymbol{n})\Big|_{\varepsilon=0} = \frac{d}{d\varepsilon}\int_{t_{1}}^{t_{2}}\int_{\omega}\rho\left(\frac{1}{2}|\mathbf{v}|^{2} - f(\phi,\mathbf{n},\nabla_{\varepsilon}\phi,\nabla_{\varepsilon}\mathbf{n})\right)d\mathbf{x}dt\Big|_{\varepsilon=0} \\
= \frac{d}{d\varepsilon}\int_{t_{1}}^{t_{2}}\int_{\Omega}\rho\left(\frac{1}{2}|\mathbf{v}|^{2} - f(\phi,\mathbf{n},\nabla_{\varepsilon}\phi,\nabla_{\varepsilon}\mathbf{n})\right)d\mathbf{X}dt\Big|_{\varepsilon=0} \\
= \frac{d}{d\varepsilon}\int_{t_{1}}^{t_{2}}\int_{\Omega}\rho_{0}\left(\frac{1}{2}|\mathbf{v}|^{2} - f(\phi,\mathbf{n},\nabla_{\varepsilon}\phi,\nabla_{\varepsilon}\mathbf{n})\right)d\mathbf{X}dt\Big|_{\varepsilon=0} \\
= \int_{t_{1}}^{t_{2}}\int_{\Omega}\rho_{0}\frac{d}{d\varepsilon}\left(\frac{1}{2}|\mathbf{v}|^{2} - f(\phi,\mathbf{n},\nabla_{\varepsilon}\phi,\nabla_{\varepsilon}\mathbf{n})\right)\Big|_{\varepsilon=0}d\mathbf{X}dt \\
= \int_{t_{1}}^{t_{2}}\int_{\omega}\rho\frac{d}{d\varepsilon}\left(\frac{1}{2}|\mathbf{v}|^{2} - f(\phi,\mathbf{n},\nabla_{\varepsilon}\phi,\nabla_{\varepsilon}\mathbf{n})\right)\Big|_{\varepsilon=0}d\mathbf{x}dt \tag{28}$$

where Ω is the domain in the initial configuration. Substituting (19-25) in the above equation and taking derivative w.r.t ϵ at $\epsilon = 0$, we find

$$\frac{dL}{d\varepsilon}\Big|_{\varepsilon=0} = \int_{t_1}^{t_2} \int_{\omega} \rho \left\{ \mathbf{v} \cdot \dot{\boldsymbol{\psi}} - \frac{\partial f}{\partial \phi} \chi - \frac{\partial f}{\partial \nabla \phi} \cdot \left(\nabla \chi - \nabla \boldsymbol{\psi} \nabla \phi \right) - \frac{\partial f}{\partial \boldsymbol{n}} \cdot \boldsymbol{\zeta} - \frac{\partial f}{\partial \nabla \boldsymbol{n}} : \left(\nabla \boldsymbol{\zeta} - \nabla \boldsymbol{\psi} \nabla \boldsymbol{n} \right) \right\} d\mathbf{x} dt$$

$$= \int_{t_1}^{t_2} \int_{\omega} \rho \left\{ \mathbf{v} \cdot \dot{\boldsymbol{\psi}} - \frac{\partial f}{\partial \phi} \chi - \frac{\partial f}{\partial \nabla \phi} \cdot \nabla \chi + \frac{\partial f}{\partial \nabla \phi} \otimes \nabla \phi : \nabla \boldsymbol{\psi} - \frac{\partial f}{\partial \boldsymbol{n}} \cdot \boldsymbol{\zeta} - \frac{\partial f}{\partial \nabla \boldsymbol{n}} : \nabla \boldsymbol{\zeta} + \frac{\partial f}{\partial \nabla \boldsymbol{n}} \nabla \boldsymbol{n}^T : \nabla \boldsymbol{\psi} \right\} d\mathbf{x} dt$$
(29)

where $\mathbf{A} : \mathbf{B} = A_{ij}B_{ij}$. Above expression can be simplified by using following identities for any scalar *a*, vector \mathbf{u} and second order tensor \mathbf{T}

$$Div(a\boldsymbol{u}) = \boldsymbol{u} \cdot \nabla a + aDiv(\boldsymbol{u}), \tag{30}$$

$$Div(\mathbf{T}\boldsymbol{u}) = \boldsymbol{u} \cdot Div(\mathbf{T}^T) + \boldsymbol{T} : \nabla \boldsymbol{u}.$$
 (31)

Using (30) and (31) in (29), we get

$$\begin{split} \frac{dL}{d\varepsilon} \bigg|_{\varepsilon=0} &= \int_{t_1}^{t_2} \int_{\omega} \rho \Big\{ (\vec{v} \cdot \vec{\psi}) - \vec{v} \cdot \psi \Big\} - \rho \frac{\partial f}{\partial \phi} \chi - \Big\{ Div \Big(\rho \chi \frac{\partial f}{\partial \nabla \phi} \Big) - \chi Div \Big(\rho \frac{\partial f}{\partial \nabla \phi} \Big) \Big\} + \Big\{ Div \Big(\rho \Big(\frac{\partial f}{\partial \nabla \phi} \otimes \nabla \phi \Big) \psi \Big) \\ &- \psi \cdot Div \Big(\rho \nabla \phi \otimes \frac{\partial f}{\partial \nabla \phi} \Big) \Big\} - \rho \frac{\partial f}{\partial n} \cdot \zeta - \Big\{ Div \Big(\rho \frac{\partial f}{\partial \nabla n} \zeta \Big) - \zeta \cdot Div \Big(\rho \frac{\partial f}{\partial \nabla n}^T \Big) \Big\} \\ &+ \Big\{ Div \Big(\rho \frac{\partial f}{\partial \nabla n} \nabla n \psi \Big) - \psi \cdot Div \Big(\rho \nabla n \frac{\partial f}{\partial \nabla n}^T \Big) \Big\} d\mathbf{x} dt. \end{split}$$

Now, by applying divergence theorem, we can simplify the above expression

$$\begin{aligned} \frac{dL}{d\varepsilon} \bigg|_{\varepsilon=0} &= \int_{t_1}^{t_2} \int_{\omega} -\rho \dot{\mathbf{v}} \cdot \boldsymbol{\psi} - \rho \frac{\partial f}{\partial \phi} \chi + \chi Div \left(\rho \frac{\partial f}{\partial \nabla \phi}\right) - \boldsymbol{\psi} \cdot Div \left(\rho \nabla \phi \otimes \frac{\partial f}{\partial \nabla \phi}\right) - \rho \frac{\partial f}{\partial \mathbf{n}} \cdot \boldsymbol{\zeta} + \boldsymbol{\zeta} \cdot Div \left(\rho \frac{\partial f}{\partial \nabla \mathbf{n}}^T\right) \\ &- \boldsymbol{\psi} \cdot Div \left(\rho \nabla \boldsymbol{n} \frac{\partial f}{\partial \nabla \mathbf{n}}^T\right) d\mathbf{x} dt - \int_{t_1}^{t_2} \int_{\partial \omega} \rho \left\{ \frac{\partial f}{\partial \nabla \phi} \chi - \left(\frac{\partial f}{\partial \nabla \phi} \otimes \nabla \phi\right) \boldsymbol{\psi} + \frac{\partial f}{\partial \nabla \mathbf{n}} \boldsymbol{\zeta} - \frac{\partial f}{\partial \nabla \mathbf{n}} \nabla \boldsymbol{n} \boldsymbol{\psi} \right\} \cdot \mathbf{N} d\mathbf{S} dt + \int_{\omega} \rho \mathbf{v} \cdot \boldsymbol{\psi} d\mathbf{x} \bigg|_{t_1}^{t_2} \\ &= -\int_{t_1}^{t_2} \int_{\omega} \left(\rho \dot{\mathbf{v}} - Div(\boldsymbol{\sigma}^E)\right) \cdot \boldsymbol{\psi} + \rho \mu \chi + \rho \mathbf{h} \cdot \boldsymbol{\zeta} d\mathbf{x} dt - \int_{t_1}^{t_2} \int_{\partial \omega} \boldsymbol{\sigma}^E \mathbf{N} \cdot \boldsymbol{\psi} + \mathbf{t} \cdot \mathbf{N} \chi + \mathbf{W} \mathbf{N} \cdot \boldsymbol{\zeta} d\mathbf{S} dt + \int_{\omega} \rho \mathbf{v} \cdot \boldsymbol{\psi} d\mathbf{x} \bigg|_{t_1}^{t_2} \end{aligned}$$

$$\tag{32}$$

where N is normal to the surface, σ^E is the elastic stress tensor,

$$\boldsymbol{\sigma}^{E} = -\rho \nabla \phi \otimes \frac{\partial f}{\partial \nabla \phi} - \rho \nabla \boldsymbol{n} \frac{\partial f}{\partial \nabla \boldsymbol{n}}^{T}, \qquad (33)$$

 μ is the generalized chemical potential and h is the elastic torque due to orientation ,

$$\mu = \frac{\partial f}{\partial \phi} - \frac{1}{\rho} Div \left(\rho \frac{\partial f}{\partial \nabla \phi} \right), \quad \text{and} \quad \boldsymbol{h} = \frac{\partial f}{\partial \boldsymbol{n}} - \frac{1}{\rho} Div \left(\rho \frac{\partial f}{\partial \nabla \boldsymbol{n}} \right)$$
(34)

 \boldsymbol{t} and \boldsymbol{W} are the generalized surface forces and

$$\boldsymbol{t} = \frac{\partial f}{\partial \nabla \phi}, \quad \text{and} \quad \boldsymbol{W} = \frac{\partial f}{\partial \nabla \boldsymbol{n}}.$$
 (35)

From (26), we have variations $\chi = 0$ and $\zeta = 0$. Since ψ, χ, ζ are compactly supported function, therefore they vanish on the surface if Dirichlet boundary conditions are provided. Also, ψ is zero if initial and final velocity is given. Finally, making variations of the functional L go to zero, we find the equilibrium equation given by

$$\rho \dot{\mathbf{v}} - Div(\boldsymbol{\sigma}^E) = 0. \tag{36}$$

Mass balance equation can be found by taking time time derivative of (27)

$$\frac{dJ\rho(\mathbf{x})}{dt} = \frac{d\rho_0(\mathbf{X})}{dt} = 0$$
$$\dot{J}\rho + \dot{\rho}J = 0$$
$$J\dot{\rho} + J\rho Div(\mathbf{v}) = 0$$
$$\dot{\rho} + \rho Div(\mathbf{v}) = 0$$

If the velocity of the two fluids are same, then the mass balance equation simplifies to

$$\nabla \cdot \boldsymbol{v} = 0. \tag{37}$$

Similarly, from (26), we have

$$\rho\phi = 0 \tag{38}$$

For the case of nematic liquid crystal, the exact form of elastic stress can be derived by substituting (17) in (33). From (17), we find

$$\frac{\partial f}{\partial \nabla \phi} = \lambda \nabla \phi + A(\boldsymbol{n} \cdot \nabla \phi) \boldsymbol{n} \quad \text{and} \quad \frac{\partial f}{\partial \nabla \boldsymbol{n}} = \frac{K(1+\phi)}{2} \nabla \boldsymbol{n}.$$
(39)

Using above expressions in (33), we get

$$\boldsymbol{\sigma}^{(E)} = -\rho \left\{ \nabla \phi \otimes \nabla \phi + \frac{K(1+\phi)}{2} \nabla \boldsymbol{n} \nabla \boldsymbol{n}^{T} - A(\boldsymbol{n} \cdot \nabla \phi) \boldsymbol{n} \otimes \nabla \phi \right\}$$
(40)

The total stress $\sigma^{(T)}$ in a nematic fluid constitutes of two terms, viscous stress $\sigma^{(V)}$ and elastic stress $\sigma^{(E)}$. Viscous stresses arise due to viscous friction between the molecules and hence doesn't depend on the nematic potential.For viscous stress $\sigma^{(V)}$ in both the components, a simple Newtonian viscous stress can be assumed. Total stress then can be written as

$$\boldsymbol{\sigma}^{(T)} = -P\boldsymbol{I} + \eta(\nabla \boldsymbol{v} + \nabla \boldsymbol{v}^T) + \boldsymbol{\sigma}^{(E)},\tag{41}$$

where η is dynamic viscosity and P is the pressure. The momentum balance equation can now be written as

$$\rho\left(\frac{\partial \boldsymbol{v}}{\partial t} + \boldsymbol{v}.\nabla \boldsymbol{v}\right) = -\nabla P + \nabla \cdot [\eta(\nabla \boldsymbol{v} + \nabla \boldsymbol{v}^T) + \boldsymbol{\sigma}^{(E)}].$$
(42)

The balance law for each component, (38), is derived by assuming no diffusion. If we have diffusion in the system then there will be diffusive flux in the system. The integral form of mass conservation for each component can be written as

$$\frac{d}{dt} \int_{\omega} \rho_i c_i d\boldsymbol{x} = -\int_{\partial \omega} \boldsymbol{J} d\boldsymbol{S} \implies \rho_i \dot{c}_i = -Div(\boldsymbol{J})$$
(43)

where J is the flux of each component, ρ_i and c_i are the density and concentration of each phase, respectively. Assuming Fick's law holds such that the flux is proportional to the gradient of the generalized potential μ , we get the Cahn-Hilliard equation for the nematic liquid crystal as

$$\rho_1 \dot{\phi} = \nabla \cdot \left(\rho_1 \gamma_1 \nabla \mu \right) \implies \dot{\phi} = \gamma_1 \nabla^2 \mu, \tag{44}$$

where γ_1 is the mobility which is taken to be constant. Relaxation time of the phase field ϕ is proportional to $1/\gamma_1$. When γ_1 tends to zero, the equation reduces to the kinematic free surface condition. Using (17), we find

$$\frac{\partial f}{\partial \phi} = \lambda \frac{\phi(\phi^2 - 1)}{\epsilon^2} + \frac{1}{2} f_{bulk}, \text{ and } \frac{\partial f}{\partial \nabla \phi} = \lambda \nabla \phi + A(\boldsymbol{n} \cdot \nabla \phi) \boldsymbol{n}.$$
 (45)

Therefore from (34), we obtain

$$\mu = \lambda \left[\frac{\phi(\phi^2 - 1)}{\epsilon^2} - \nabla^2 \phi \right] + \frac{1}{2} f_{bulk} - A \nabla \cdot \left[(\boldsymbol{n} \cdot \nabla \phi) \boldsymbol{n} \right].$$
(46)

The director n can rotate due to elastic torque and viscous torque in the system. The elastic torque, h, is due to free energy of the system and is given by (34). Using (17), we get

$$\frac{\partial f}{\partial \boldsymbol{n}} = \frac{K(1+\phi)}{2} \frac{(|\boldsymbol{n}|^2 - 1)\boldsymbol{n}}{\delta^2} + A(\boldsymbol{n} \cdot \nabla \phi) \nabla \phi \quad \text{and} \quad \frac{\partial f}{\partial \nabla \boldsymbol{n}} = K \frac{(1+\phi)}{2} \nabla \boldsymbol{n}, \tag{47}$$

which when substituted in (34) gives

$$\boldsymbol{h} = K \left[\frac{(1+\phi)}{2} \frac{(|\boldsymbol{n}|^2 - 1)\boldsymbol{n}}{\delta^2} - \nabla \cdot \frac{(1+\phi)}{2} \nabla \boldsymbol{n} \right] + A(\boldsymbol{n} \cdot \nabla \phi) \nabla \phi.$$
(48)

Neglecting viscous torque, the director equation can be written as

$$\dot{\boldsymbol{n}} = \gamma_2 \boldsymbol{h},\tag{49}$$

where γ_2 represents the relaxation time of the director. The viscous effects are neglected in the director equation because of two reasons. First, the only effect of viscous forces is to slow down the evolution process which is governed by conservative forces. Second, it increases the computation time and complexity unnecessarily. The Equations (37),(42),(44) and(49) gives the complete set of equations for binary mixture of Newtonian and nematic fluid which can be solved with appropriate boundary conditions.

3 Numerical scheme

We have derived four sets of equations for four variables ϕ , n, v and P. However, they are coupled nonlinear equations and are not easy to solve numerically. To simplify the equations we write them as

$$\frac{\partial \boldsymbol{v}}{\partial t} - \nu \Delta \boldsymbol{v} + \Delta P = \boldsymbol{h}_1 \tag{50}$$

$$\nabla \cdot \boldsymbol{v} = 0, \tag{51}$$

$$\frac{\partial\phi}{\partial t} + \gamma_1 \lambda \Delta^2 \left(\Delta^2 \phi - \frac{(|\phi|^2 - 1)\phi}{\epsilon^2} \right) = h_2, \tag{52}$$

$$\frac{\partial \boldsymbol{n}}{\partial t} + \frac{\gamma_2 K}{2} \left(\nabla^2 \boldsymbol{n} - \frac{(|\boldsymbol{n}|^2 - 1)\boldsymbol{n}}{\delta^2} \right) = \boldsymbol{h}_3, \tag{53}$$

where h_1, h_2 and h_3 includes all the nonlinear terms. Now, we will apply the semi-implicit second-order scheme on the linear non-coupled equations and the non-linear terms will be treated separately. For the Cahn-Hilliard equation (52), the standard semi-implicit scheme leads to a very stiff system when $\epsilon << 1$ and hence a shifted semi-implicit scheme is applied which is more stable. The discretization using shifted semi-implicit scheme results in

$$\frac{3\phi^{k+1} - 4\phi^k + \phi^{k-1}}{2\Delta t} + \gamma_1 \lambda \left(\Delta^2 - \frac{C_s}{\epsilon^2}\Delta\right)\phi^{k+1} + \frac{\gamma_1\lambda}{\epsilon^2}\Delta \left[2(|\phi^k|^2 - 1(1+C_s))\phi^k - (|\phi^{k-1}|^2 - 1(1+C_s))\phi^{k-1}\right] = 2h_1^k - h_1^{k-1},$$
(54)

where C_s is a stabilizing parameter which varies between 1 to 5. Above equation is a fourth order differential equation with constant coefficients. Similar discretization can be done for the director equation (53). For solving the stokes-problem (50) and (51) a brief approach for different boundary conditions is described in [6].

Conclusion

An energetic variational formulation using phase variables ϕ and n is done for a nematic- Newtonian fluid blend. The free energy of the blend can be expressed as the sum of mixing energy in the interfacial region, distortion energy of the nematic crystals in the bulk, and anchoring energy at the surface. In the absence of dissipation, a Lagrangian (L = T - V) can be written using the free energy. Making the first variation of the functional go to zero, we can find the linear momentum equation for the system. The mass balance for the blend is given by the constraint that relates density in the current configuration with the density in the initial configuration. The mass balance for each component includes both the advection and diffusion terms. The effect of diffusion can be included by assuming the generalized form of Fick's law which states that the diffusion is proportional to the generalized chemical potential. This leads to the classical Cahn-Hilliard equation for diffusion. The elastic stress tensor in the fluid is given by the first variation of lagrangian L, and the viscous stress tensor is assumed to be of the type Newtonian. The torque on the director includes both elastic and viscous torque. Neglecting the effects of viscous torque, the director equation can be found by using elastic torque obtained from variations of L. The final set of equations is nonlinear and coupled. To solve these, we segregate the linear and nonlinear parts, which is then solved using shifted semi-implicit scheme.

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Figures



Figure 1: A double well potential. Source:Google



Figure 2: Plot of ϕ vs \hat{x}



Figure 3: Different states of distortion. Source [7]

Tables