Variational Modeling and Complex Fluids

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Abstract

In this chapter, a general energetic variational framework for modeling the dynamics of complex fluids is introduced. The approach reveals and focuses on the couplings and competitions between different mechanisms involved for specific materials, including energetic contributions vs. kinematic transport relations, conservative parts vs. dissipative parts and kinetic parts vs. free energy parts of the systems, macroscopic deformation or flows vs. microscopic deformations, bulk effects vs. boundary conditions, etc. One has to notice that these variational approaches are motivated by the seminal works of Rayleigh (Proc Lond Math Soc 1(1):357–368, 1871) and Onsager (Phys Rev 37(4):405, 1931; Phys Rev 38(12):2265, 1931). In this chapter, the underlying physical principles and background, as well as the limitations of these approaches, are demonstrated. Besides the classical models for ideal fluids and elastic solids, these approaches are employed for models of viscoelastic fluids, diffusion, and mixtures.

1 Introduction

The focus of this chapter is on the mathematical modeling of anisotropic complex fluids whose motion is complicated by the existence of mesoscales or subdomain structures and interactions. These complex fluids are ubiquitous in daily life, including wide varieties of mixtures, polymeric solutions, colloidal dispersions, biofluids, electro-rheological fluids, ionic fluids, liquid crystals, and liquid-crystalline polymers. On the other hand, such materials often have great practical utility since the microstructure can be manipulated by external field or forces in order to produce useful mechanical, optical, or thermal properties. An important way of utilizing complex fluids is through composites of different materials. By blending two or more different components together, one may derive novel or enhanced properties from the composite. The properties of composites may be tuned to suit a particular application by varying the composition, concentration, and, in many situations, the phase morphology. One such composite is polymer blends [121]. Under optimal processing conditions, the dispersed phase is stretched into a fibrillar morphology. Upon solidification, the long fibers act as reinforcement and impart great strength to the composite. The effect is particularly strong if the fibrillar phase is a liquid-crystalline polymer [99]. Another example is polymer-dispersed liquid crystals, with liquid crystal droplets embedded in a polymer matrix, which have shown great potential in electro-optical applications [127].

Unlike solids and simple liquids, the model equations for complex fluids continue to evolve as new experimental evidences and applications become available [97]. The complicated phenomena and properties exhibited by these materials reflect the coupling and competition between the microscopic interactions and the macroscopic dynamics. New mathematical theories are needed to resolve the ensemble of microelements, their intermolecular and distortional elastic interactions, their coupling to hydrodynamics, and the applied electric or magnetic fields. The most

common origin and manifestation of anomalous phenomena in complex fluids are different "elastic" effects [77]. They can be attributed to the elasticity of deformable particles; elastic repulsion between charged liquid crystals, polarized colloids, and multicomponent phases; elasticity due to microstructures; or bulk elasticity endowed by polymer molecules in viscoelastic complex fluids. These elastic effects can be represented in terms of certain internal variables, for example, the orientational order parameter in liquid crystals (related to their microstructures), the distribution density function in the dumbbell model for polymeric materials, the magnetic field in magnetohydrodynamic fluids, the volume fraction in mixture of different materials, etc. The different rheological and hydrodynamic properties will be attributed to the special coupling (interaction) between the transport (macroscopic fluid motions) of the internal variable and the induced (microscopic) elastic stress [115, 116]. This coupling gives not only the complicated rheological phenomena but also formidable challenges in analysis and numerical simulations of the materials.

The common feature of the systems described in this chapter is the underlying energetic variational structure. For an isothermal closed system, the combination of the first and second laws of thermodynamics yields the following energy dissipation law [6, 11, 39, 56]:

$$\frac{d}{dt} E^{\text{total}} = -\Delta, \tag{1}$$

where E^{total} is the sum of kinetic energy and the total Helmholtz free energy and Δ is the entropy production (here the rate of energy dissipation). The choices of the total energy functional and the dissipation functional, together with the kinematic (transport) relations of the variables employed in the system, determine all the physical and mechanical considerations and assumptions for the problem.

The energetic variational approaches are motivated by the seminal work of Rayleigh [106] and Onsager [100, 101]. The framework, including Least Action Principle and Maximum Dissipation Principle, provides a unique, well-defined, way to derive the coupled dynamical systems from the total energy functionals and dissipation functions in the dissipation law (1) [67]. Instead of using the empirical constitutive equations, the force balance equations are *derived*. Specifically, the Least Action Principle (LAP) determines the Hamiltonian part of the system [2, 5, 50], and the Maximum Dissipation Principle (MDP) accounts for the dissipative part [11, 101]. Formally, LAP represents the fact that force multiplies distance is equal to the work, i.e., $\delta E = \text{force} \times \delta x$, where x is the location and δ the variation/derivative. This procedure gives the Hamiltonian part of the system and the conservative forces [2, 5]. The MDP, by Onsager and Rayleigh [67, 100, 101, 106], produces the dissipative forces of the system, $\delta \frac{1}{2} \Delta = \text{force} \times \delta \dot{x}$. The factor $\frac{1}{2}$ is consistent with the choice of quadratic form for the "rates" that describe the linear response theory for longtime near-equilibrium dynamics [74]. The final system is the result of the balance of all these forces (Newton's Second Law).

Both total energy and energy dissipation may contain terms related to microstructure and those describing macroscopic flow. Competition between different parts

of energy, as well as energy dissipation, defines the dynamics of the system. The main goal of this chapter is on describing the role of microstructures in the special coupling between the kinematic transport and the induced "elastic" stresses.

2 Nonequilibrium Thermodynamics

In this section, some basic thermodynamic principles and general relations between energy laws and differential equations are described. We first clarify notation of variations of the functionals [50, 54]. Let $\mathcal{E} = \mathcal{E}(\psi)$ be a functional depending on a function ψ in a space H which is equipped with an inner product $\langle \ , \ \rangle_H$. The variation $\delta\mathcal{E} = \delta_\psi\mathcal{E}$ of a function $\mathcal{E}$ is defined as

$$\delta_\psi\mathcal{E}(\psi) = \lim_{h \to 0} \left[\mathcal{E}(\psi + h\delta\psi) - \mathcal{E}(\psi)\right]/h,$$

where $\delta\psi$ is a function so that $\psi + h\delta\psi$ is a variation of ψ. The quantity $\delta_\psi\mathcal{E}$ is often called a directional derivative in the direction of $\delta\psi$ at ψ. It is formally the Gâteau derivative of $\mathcal{E}$ at ψ in the direction of $\delta\psi$. If $\delta_\psi\mathcal{E}$ can be written as

$$\delta_\psi\mathcal{E}(\psi) = \langle f, \delta\psi \rangle_H,$$

with some f for a big class of $\delta\psi$, we often write f by

$$H_-\frac{\delta\mathcal{E}}{\delta\psi} \quad \text{or simply} \quad \frac{\delta\mathcal{E}}{\delta\psi}.$$

This quantity corresponds to the total derivative or the Fréchet derivative if the latter is well defined [55]. It is simply called the variational derivative . In this notation, denominator points to the function with respect to which the variation of the functional in the numerator is taken.

2.1 Energetic Variational Approaches

The first law of thermodynamics [56] states that the rate of change of the sum of kinetic energy $\mathcal{K}$ and the internal energy $\mathcal{U}$ can be attributed to either the work $\dot{W}$ done by the external environment or the heat $\dot{Q}$:

$$\frac{d}{dt}(\mathcal{K} + \mathcal{U}) = \dot{W} + \dot{Q}.$$

In other words, the first law of thermodynamics is really the law of conservation of energy. It is noticed the internal energy describes all the interactions in the system. In order to analyze heat, one needs to introduce the entropy $\mathcal{S}$ [56], which naturally leads to the second law of thermodynamics [39, 56]:

$$T\frac{d\mathcal{S}}{dt} = \dot{Q} + \Delta$$

where T is the temperature and $\mathcal{S}$ is the entropy. Δ is the entropy production which is always nonnegative and gives the rate of energy dissipation in irreversible systems. Subtracting the two laws, in the isothermal case when T is constant, one arrives at:

$$\frac{d}{dt}(\mathcal{K} + \mathcal{U} - T\mathcal{S}) = \dot{W} - \Delta,$$

where $\mathcal{F} = \mathcal{U} - T\mathcal{S}$ is called the Helmholtz free energy. We denote $E^{\text{total}} = \mathcal{K} + \mathcal{F}$ to be total energy of the system. If the system is closed, when work done by the environment $\dot{W} = 0$, the energy dissipation law of the system can be written as

$$\frac{dE^{\text{total}}}{dt} = -2\mathcal{D}. \tag{2}$$

The quantity $\mathcal{D} = \frac{1}{2}\Delta$ is sometimes called the energy dissipation. The dissipative law allows one to distinguish two types of systems: conservative (or Hamiltonian) and dissipative.

The choices of the total energy components and the energy dissipation take into consideration all the physics of the system and determine the dynamics through the two distinct variational processes: Least Action Principle (LAP) and Maximum Dissipation Principle (MDP).

To derive the differential equation describing the conservative system ($\Delta = 0$), one employs the Least Action Principle (LAP) [2, 5], which says that the dynamics is determined as a critical point of the action functional (Remark 1 below). We give its equivalent form. We consider functionals $\int_0^T \mathcal{K}dt$ and $\int_0^T \mathcal{F}dt$ defined for a function $\mathbf{x}$ (the trajectory in Lagrangian coordinates, if applicable) depending on space time variables. The inertial and conservative force from the kinetic and free energies are, respectively, defined as

$$\text{force}_{\text{inertial}} = H\_\frac{\delta \int_0^T \mathcal{K}dt}{\delta \mathbf{x}},$$

$$\text{force}_{\text{conservative}} = H\_\frac{\delta \int_0^T \mathcal{F}dt}{\delta \mathbf{x}}.$$

The space H is typically taken as the space time L^2 space, $L_{x,t}^2$, i.e., $L_{x,t}^2 = L^2(0, T; L_x^2)$, where L_x^2 is the L^2 space in the spatial variables. (These are called variational forces.) In other words, for all $\delta\mathbf{x}$,

$$\delta\int_0^T \mathcal{K}dt = \langle \text{force}_{\text{inertial}}, \delta\mathbf{x}\rangle_{L_{x,t}^2} = \int_0^T \langle \text{force}_{\text{inertial}}, \delta\mathbf{x}\rangle_{L_x^2}dt$$

$$\delta\int_0^T \mathcal{F}dt = \langle \text{force}_{\text{conservative}}, \delta\mathbf{x}\rangle_{L_{x,t}^2} = \int_0^T \langle \text{force}_{\text{conservative}}, \delta\mathbf{x}\rangle_{L_x^2}dt.$$

The LAP can be written as

$$\delta \int_0^T \mathcal{K} dt = \delta \int_0^T \mathcal{F} dt$$

for all $\delta \mathbf{x}$. This gives the natural variational form (the weak form) of the forces with suitable test functions $\delta \mathbf{x}$. The strong form of the system (Euler-Lagrange equation) can be also written as a force balance (without dissipation).

$$\text{force}_{\text{inertial}} = \text{force}_{\text{conservative}}. \tag{3}$$

The inertial force corresponds to the inertial term ma in Newton's Second Law, where a is the acceleration and m is the mass. Note that if the variation is performed on a bounded domain and involves integration by parts, one has to assume specific boundary conditions to cancel the boundary terms, so that no boundary effects are involved.

Remark 1. The standard approach [5] dictates to define the Lagrangian functional $\mathcal{L} = \mathcal{K} - \mathcal{F}$ and the action functional as $\mathcal{A}(\mathbf{x}) = \int_0^T \mathcal{L} dt$. The Euler-Lagrange equation in this case is $H \_ \frac{\delta \mathcal{A}}{\delta \mathbf{x}} = 0$.

For a dissipative system ($\Delta = 2\mathcal{D} > 0$), according to Onsager [100, 101], the dissipation $\mathcal{D}$ is taken to be proportional to a "rate" $\mathbf{x}_t$ raised to a second power. The Maximum Dissipation Principle (MDP) [67] implies that the dissipative force may be obtained by minimization of the dissipation functional $\mathcal{D}$ with respect to the above mentioned "rate." Hence, through MDP, the dissipative force (linear with respect to the same rate function) can be derived as follows:

$$\delta \mathcal{D} = \langle \text{force}_{\text{dissipative}}, \delta \mathbf{x}_t \rangle_{\tilde{H}}.$$

In other words,

$$\tilde{H} \_ \delta \mathcal{D}/\delta \mathbf{x}_t = \text{force}_{\text{dissipative}}.$$

Note that the test function in MDP is different from that in LAP before.

Remark 2. It is important to note that although the limitation for the dissipation $\mathcal{D}$ to be quadratic in "rate" is rather restrictive, strong nonlinearities can be introduced through coefficients independent of the "rate."

When all forces are derived, according to the force balance (Newton's Second Law, where inertial force plays role of ma):

$$\text{force}_{\text{inertial}} = \text{force}_{\text{conservative}} + \text{force}_{\text{dissipative}}. \tag{4}$$

Notation. *For shorter notation, one can write Eq.* (4) *as* $H_-\frac{\delta \int_0^T \mathcal{K}dt}{\delta \mathbf{x}} =$ $H_-\frac{\delta \int_0^T \mathcal{F}dt}{\delta \mathbf{x}} + \tilde{H}_-\frac{\delta \mathcal{D}}{\delta \mathbf{x}_t}$ *with* $H = L^2(0, T; \tilde{H})$.

It is important to notice that Eq. (4) uses the strong form of the variational result. This might bring ambiguity in the original variational weak form, since the test functions may be in different spaces.

2.2   Hookean Spring

As a start, a simple ordinary differential equations (ODE) example of a dissipative system is considered here, which had been originally proposed by Lord Rayleigh [106]: the Hookean spring of which one end is attached to the wall and the other end to a mass m (see Fig. 1). Let $x(t)$ be a displacement of the mass from the equilibrium. Consider that the spring has friction-based damping which is proportional to the velocity (relative friction to the resting media). Under these assumptions,

$$\mathcal{K} = \frac{mx_t^2}{2}, \quad \mathcal{F} = \frac{kx^2}{2}, \text{ and } \quad \mathcal{D} = \frac{\gamma x_t^2}{2},$$

where k is spring strength material parameter and γ is damping coefficient. The energy dissipation law is clearly as follows:

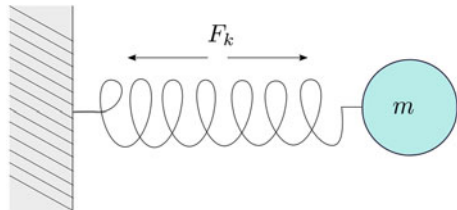$$\frac{d}{dt}\left(\frac{mx_t^2}{2} + \frac{kx^2}{2}\right) = -\gamma x_t^2.$$

The corresponding action functional of the spring [50] in terms of the position $x(t)$:

$$\mathcal{A} = \int_0^T \left(\frac{mx_t^2}{2} - \frac{kx^2}{2}\right) dt.$$

Then the Least Action Principle, i.e., variation with respect to the trajectory $x(t)$, yields [50]:

Fig. 1 Spring attached to a wall on one end, with mass m on the other end

$$\delta \mathcal{A} = \int_0^T [mx_t (\delta x)_t - kx\delta x] \, dt = \int_0^T (-mx_{tt} - kx) \, \delta x \, dt$$

$$= \left\langle L_{t-}^2 \frac{\delta \mathcal{A}}{\delta x}, \delta x \right\rangle_{L^2(0,T)} = \int_0^T \left\langle L_{t-}^2 \frac{\delta \mathcal{A}}{\delta x}, \delta x \right\rangle_{\mathbf{R}} \, dt.$$

Here the space H with inner product is $L_t^2 = L^2(0, T)$ because here L_x^2 is just $\mathbb{R}$. On the other hand, the principle of maximum dissipation gives

$$\mathbb{R}_- \frac{\delta \mathcal{D}}{\delta x_t} = \gamma x_t.$$

Indeed, looking at forces involved and formulating Newton's Second Law ($F = ma$) for this system, one can get $mx_{tt} = -kx - \gamma x_t$, or equivalently

$$mx_{tt} + \gamma x_t + kx = 0, \tag{5}$$

which is equivalent to the variational force balance (corresponding to (4)) $L_{t-}^2 \frac{\delta \mathcal{A}}{\delta x} = \mathbb{R}_- \frac{\delta \mathcal{D}}{\delta x_t}$ for this example.

Looking at the explicit solution of (5), it is clear that the Hamiltonian part describes the transient dynamics, the oscillation near initial data, while the dissipative part gives the decaying longtime behavior near equilibrium.

2.3   Gradient Flow (Dynamics of Fastest Descent)

The energetic variational approaches have many different forms in practices and applications. Next look at the familiar example of gradient flow (dynamics of fastest descent):

$$\gamma \frac{\delta \mathcal{F}(\varphi)}{\delta \varphi} + \varphi_t = 0, \tag{6}$$

where $\mathcal{F}$ is a general energy functional in terms of φ. Here φ is a function of spatial variables with parameter time t, and the constant $\gamma > 0$ is the dissipation rate which determines the evolution approaching the equilibrium. Such a system has been used in many applications both in physics and in mathematics; in particular, it is commonly used in both analysis and numerics to achieve the minimum of a given energy functional.

It is clear that with natural boundary conditions (Dirichlet or Neumann), the solution of (6) satisfies the following energy dissipation law (by chain rule and integration by parts, if needed):

$$\frac{d}{dt} \mathcal{F} = -\int_\Omega \frac{1}{\gamma} |\varphi_t|^2 \, d\mathbf{x},$$

where Ω is a domain in a Euclidean space.

On the other hand, one can put this in the general framework of energetic variational approaches. Notice that there is no kinetic energy in this system, indicating the nature of being the longtime near-equilibrium dynamics.

Notation. *When working on a bounded domain, one should consider a variation up to the boundary. Generally, for a functional $\mathcal{E}$ depending on a function ψ defined in Ω, the variation $\delta_\psi \mathcal{E}$ is often of the form*

$$\delta_\psi \mathcal{E}(\psi) = \int_\Omega f \delta\psi \, d\mathbf{x} + \int_{\partial\Omega} g \delta\psi \, dS.$$

Then, we denote

$$f = \frac{\delta\mathcal{E}}{\delta_\Omega \psi}, \quad g = \frac{\delta\mathcal{E}}{\delta_{\partial\Omega} \psi}.$$

Here f gives variational force inside the domain, while g is a kind of a boundary force. So if the boundary is taken into account, boundary forces should be also balanced.

Unless mentioned otherwise, in this chapter, specific boundary conditions are taken to cancel the boundary effects (i.e., make boundary integral equal to zero).

In the case of $\mathcal{F} = \int_\Omega W(\varphi, \nabla_\mathbf{x}\varphi) \, d\mathbf{x}$ and $\mathcal{D} = \frac{1}{2\gamma} \int_\Omega |\varphi_t|^2 d\mathbf{x}$, the variation leads to the following two variational derivatives:

$$L^2_{\mathbf{x}-}\frac{\delta\mathcal{F}}{\delta_\Omega\varphi} = -\nabla \cdot \frac{\partial W}{\partial\nabla\varphi} + \frac{\partial W}{\partial\varphi}, \quad L^2_{\mathbf{x}-}\frac{\delta\mathcal{D}}{\delta_\Omega\varphi_t} = \frac{1}{\gamma}\varphi_t,$$

which after substitution in (4) yield equation (6). In this case, the boundary effects would be canceled out in case of homogeneous Dirichlet or Neumann boundary conditions.

Remark 3. To derive implicit Euler's time discretization scheme [8], one may consider minimization of the following functional:

$$\min_{\substack{\varphi^{n+1} \\ \text{given } \varphi^n}} \int_\Omega \left\{ \frac{1}{\gamma} \frac{|\varphi^{n+1} - \varphi^n|^2}{2\Delta t} + W\left(\varphi^{n+1}, \nabla\varphi^{n+1}\right) \right\} d\mathbf{x}.$$

By introducing time discretization, one can avoid the two different variations and only take the variation with respect to φ^{n+1}. However, the scheme often fails in the case of γ dependent on φ, since it is unclear whether to take it explicit or implicit: explicit may cause stability issues and implicit will lead to a highly nonlinear system.

3 Basic Mechanics

Before moving on to more complicated and realistic applications, it is important first to introduce some basic terminologies and concepts in continuum mechanics [36,59]. In particular, in this section, the relation between Eulerian (space reference) and Lagrangian (material reference) coordinates [119] is explored, and the variational techniques in terms of deformable medium are described. In this section, the boundary conditions are not in the focus of attention. However they may and should also be derived through the variational procedure with various specific boundary energy terms and dissipative terms.

3.1 Flow Map and Deformation Gradient

For a given velocity field $\mathbf{u}(\mathbf{x}, t)$, one can define the corresponding flow map (trajectory) $\mathbf{x}(\mathbf{X}, t)$ as

$$\mathbf{x}_t = \mathbf{u}, \quad \mathbf{x}(\mathbf{X}, 0) = \mathbf{X}. \tag{7}$$

In other words, $\mathbf{x}(\mathbf{X}, t)$ describes the position of a particle moving with velocity $\mathbf{u}$ and initial position $\mathbf{X}$. Here $\mathbf{x}$ are the Eulerian coordinates, and $\mathbf{X}$ – the Lagrangian coordinates or initial configuration (see Fig. 2). Since the flow map should satisfy (7), its recovery is possible only if $\mathbf{u}(\mathbf{x}, t)$ has certain regularity properties, for instance, being Lipschitz in $\mathbf{x}$ [36].

In order to describe the evolution of structures or patterns (configurations), it is clear that one needs to consider the matrix of partial derivatives, the Jacobian matrix, the deformation gradient (or deformation tensor) [61]:

$$F(\mathbf{X}, t) = \frac{\partial \mathbf{x}(\mathbf{X}, t)}{\partial \mathbf{X}}.$$

If one writes F by components (F_{ij}), our convention is

$$F_{ij} = \frac{\partial x_i}{\partial X_j}.$$

Fig. 2 A schematic illustration of a flow map $\mathbf{x}(\mathbf{X}, t)$. For t fixed $\mathbf{x}$ maps $\Omega_{\mathbf{X}}^0$ to $\Omega_{\mathbf{x}}^t$. For $\mathbf{X}$ fixed $\mathbf{x}(\mathbf{X}, t)$ is the trajectory of $\mathbf{X}$
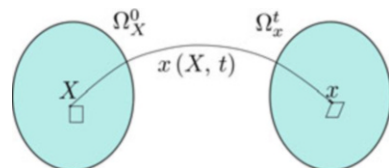
Then by chain rule:

$$\frac{\partial F_{ij}}{\partial t} = \frac{\partial}{\partial t}\left(\frac{\partial x_i}{\partial X_j}\right) = \frac{\partial}{\partial X_j}\left(\frac{\partial x_i}{\partial t}\right) = \frac{\partial}{\partial X_j}u_i\left(\mathbf{x}\left(\mathbf{X}, t\right), t\right) = \sum_k \frac{\partial u_i}{\partial x_k}\frac{\partial x_k}{\partial X_j},$$

which in Eulerian coordinates will take the form as:

$$\tilde{F}_t + (\mathbf{u} \cdot \nabla_\mathbf{x})\,\tilde{F} = \frac{\partial F}{\partial t} = \frac{\partial}{\partial \mathbf{X}}\mathbf{u}\left(\mathbf{x}\left(\mathbf{X}, t\right), t\right) = (\nabla_\mathbf{x}\mathbf{u})\,\tilde{F}.$$

Here $\tilde{F}\left(\mathbf{x}\left(\mathbf{X}, t\right), t\right) = F\left(\mathbf{X}, t\right)$ and $\nabla_\mathbf{x}$ denote the gradient. In Eulerian coordinates, $\tilde{F}$ satisfies the following important identity:

$$\tilde{F}_t + (\mathbf{u} \cdot \nabla_\mathbf{x})\,\tilde{F} = (\nabla_\mathbf{x}\mathbf{u})\,\tilde{F}. \tag{8}$$

Remark 4. The form of (8) is directly related to the equation of vorticity $\mathbf{w} = \mathrm{curl}\,\mathbf{u}$ in inviscid incompressible fluids [94]: in two-dimensional cases, the solution of $w_t + (\mathbf{u} \cdot \nabla)\,w = 0$ is expressed along the trajectory as $w\left(\mathbf{x}\left(\mathbf{X}, t\right), t\right) = w_0\left(\mathbf{X}\right)$; in three-dimensional case $\mathbf{w}_t + (\mathbf{u} \cdot \nabla)\,\mathbf{w} - (\mathbf{w} \cdot \nabla)\,\mathbf{u} = 0$, the solution becomes $\mathbf{w}\left(\mathbf{x}\left(\mathbf{X}, t\right), t\right) = F\mathbf{w}_0\left(\mathbf{X}\right)$. It is clear that the stretch term $(\mathbf{w} \cdot \nabla)\mathbf{u}$ is the direct consequence of the deformation F, although F itself is absent from the original fluid equations.

Remark 5. Incompressibility condition is actually a restriction on deformation $\det F = 1$. By using Jacobi's formula,

$$0 = \partial_t \det F = \det F \cdot \mathrm{tr}\left(F^{-1}\partial_t F\right) = 1 \cdot \mathrm{tr}\left(\frac{\partial \mathbf{X}}{\partial \mathbf{x}}\frac{\partial \mathbf{u}}{\partial \mathbf{X}}\right) = \mathrm{tr}\left(\nabla_\mathbf{x}\mathbf{u}\right) = \nabla_\mathbf{x} \cdot \mathbf{u},$$

which yields the usual incompressibility condition in conventional descriptions of fluids. Notice that the nonlinear constraint in Lagrangian coordinates becomes a linear one in Eulerian coordinates. (Here $\nabla_\mathbf{x} \cdot \mathbf{u}$ denotes the divergence of $\mathbf{u}$.)

Remark 6. F also determines the kinematic relations of transport of various physical quantities. The following formulations of kinematic relations describing transport of scalar quantities are expressed in Eulerian and Lagrangian coordinates as:

$$\varphi_t + (\mathbf{u} \cdot \nabla_\mathbf{x})\,\varphi = 0 \text{ is equivalent to } \varphi\left(\mathbf{x}\left(\mathbf{X}, t\right), t\right) = \varphi\left(\mathbf{X}, 0\right), \tag{9}$$

$$\varphi_t + \nabla_\mathbf{x} \cdot (\varphi\mathbf{u}) = 0 \text{ is equivalent to } \varphi\left(\mathbf{x}\left(\mathbf{X}, t\right), t\right) = \frac{\varphi\left(\mathbf{X}, 0\right)}{\det F}. \tag{10}$$

3.2 Newtonian Fluids and Navier-Stokes Equations

Next the classic Newtonian fluids [36] are examined, and the Navier-Stokes equations are derived from the energetic variational approaches. Consider fluid with density ρ and velocity field $\mathbf{u}$. Here the local mass conservation law is postulated, i.e.,

$$\rho_t + \nabla_{\mathbf{x}} \cdot (\rho \mathbf{u}) = 0. \tag{11}$$

For fluids, one should consider the free energy depending only on the density ρ (the single most important characterization of the material being a fluid), which implies the following energy dissipation law:

$$\frac{d}{dt} \int_\Omega \left[\frac{\rho |\mathbf{u}|^2}{2} + \omega(\rho) \right] d\mathbf{x} = -\int_\Omega \left[2\eta \left| \frac{\nabla \mathbf{u} + (\nabla \mathbf{u})^T}{2} \right|^2 + \left(\zeta - \frac{2}{3}\eta \right) |\nabla \cdot \mathbf{u}|^2 \right] d\mathbf{x}, \tag{12}$$

where $\left| \frac{\nabla \mathbf{u} + (\nabla \mathbf{u})^T}{2} \right|^2 = \sum_{i,j} \frac{(u_{i,j} + u_{j,i})^2}{2}$, $u_{i,j} = \partial u_i / \partial x_j$. In general for matrix M, we write $|M| = \sqrt{\mathrm{tr} M M^T}$ which is often called the Hilbert-Schmidt norm or the Frobenius norm. Then $\mathcal{K} = \int_\Omega \frac{\rho |\mathbf{u}|^2}{2} d\mathbf{x}$, $\mathcal{F} = \int_\Omega \omega(\rho) d\mathbf{x}$, $\mathcal{D} = \int_\Omega \left[\eta \left| \frac{\nabla \mathbf{u} + (\nabla \mathbf{u})^T}{2} \right|^2 + (\frac{1}{2}\zeta - \frac{1}{3}\eta) |\nabla \cdot \mathbf{u}|^2 \right] d\mathbf{x}$. The last being the viscosity contribution [76], the relative friction between particles of the fluids. The constants η and ζ are called coefficients of viscosity (ζ is second viscosity coefficient), and $\omega(\rho)$ is free energy density.

Since the rate in the dissipation is $\mathbf{u} = \mathbf{x}_t$, one will have to take the variation with respect to the flow map $\mathbf{x}$ in the Lagrangian coordinates $\mathbf{X}$. Since $d\mathbf{x} = (\det F)\mathbf{X}$, and since (11) and (10) imply $\rho(\mathbf{x}(\mathbf{X}, t), t) = \rho_0(\mathbf{X}) / \det F(\mathbf{X}, t)$ with $\rho_0(\mathbf{X}) = \rho(\mathbf{X}, 0)$, we observe that

$$
\begin{aligned}
\delta \int_0^T \mathcal{K} dt &= \delta \int_0^T \int \frac{1}{2} \frac{\rho_0(\mathbf{X})}{\det F} |\mathbf{x}_t(\mathbf{X}, t)|^2 \det F d\mathbf{X} dt = \delta \int_0^T \int \frac{1}{2} \rho_0(\mathbf{X}) |\mathbf{x}_t(\mathbf{X}, t)|^2 d\mathbf{X} dt \\
&= \int_0^T \int \rho_0 \mathbf{x}_t \cdot \delta \mathbf{x}_t d\mathbf{X} dt = -\int_0^T \int \rho_0 \mathbf{x}_{tt} \cdot \delta \mathbf{x} d\mathbf{X} dt \\
&= \int_0^T \int \left[-\rho \frac{d}{dt} \mathbf{u}(\mathbf{x}(\mathbf{X}, t), t) \cdot \delta \mathbf{x} \right] d\mathbf{x} dt \\
&= \int_0^T \int \left[-\rho (\mathbf{u}_t + (\mathbf{u} \cdot \nabla) \mathbf{u}) \cdot \delta \mathbf{x} \right] d\mathbf{x} dt = \langle -\rho (\mathbf{u}_t + (\mathbf{u} \cdot \nabla_x)\mathbf{u}), \delta \mathbf{x} \rangle_{L^2_{\mathbf{x},t}},
\end{aligned}
$$

$$
\begin{aligned}
\delta \int_0^T \mathcal{F} dt &= \delta \int_0^T \int \omega \left(\frac{\rho_0}{\det F} \right) \det F d\mathbf{X} dt \\
&= \int_0^T \int \left[-\omega_\rho \left(\frac{\rho_0}{\det F} \right) \frac{\rho_0}{\det F} + \omega \left(\frac{\rho_0}{\det F} \right) \right] \det F \, \mathrm{tr} \left(F^{-1} \frac{\partial \delta \mathbf{x}}{\partial \mathbf{X}} \right) d\mathbf{X} dt \\
&= \int_0^T \int \left[-\omega_\rho(\rho) \rho + \omega(\rho) \right] (\nabla_{\mathbf{x}} \cdot \delta \mathbf{x}) d\mathbf{x} dt \\
&= \int_0^T \int \nabla_{\mathbf{x}} \left[\omega_\rho(\rho) \rho - \omega(\rho) \right] \cdot \delta \mathbf{x} \, d\mathbf{x} dt = \langle \nabla \left[\omega_\rho(\rho)\rho - \omega(\rho) \right], \delta \mathbf{x} \rangle_{L^2_{\mathbf{x},t}}.
\end{aligned}
$$

The normal component of the variation $\delta\mathbf{x} \cdot \nu$ is assumed to be zero at the boundary $\partial\Omega$, which follows from no penetration boundary condition. This gives the following force terms expressed in the strong PDE form:

$$L_{\mathbf{x},t-}^2 \frac{\delta \int_0^T \mathcal{K} dt}{\delta_\Omega \mathbf{x}} = -\rho \left(\mathbf{u}_t + (\mathbf{u} \cdot \nabla) \mathbf{u}\right), \quad L_{\mathbf{x},t-}^2 \frac{\delta \int_0^T \mathcal{F} dt}{\delta_\Omega \mathbf{x}} = \nabla \left[\omega_\rho(\rho)\rho - \omega(\rho)\right],$$

The second (conservative) force term is exactly the gradient of the thermodynamic pressure. In the absence of the dissipation, from the force balance (3) with LAP, one obtains the compressible Euler equations [118]:

$$\begin{cases} \rho_t + \nabla \cdot (\rho\mathbf{u}) = 0, \\ \rho\left(\mathbf{u}_t + (\mathbf{u} \cdot \nabla)\mathbf{u}\right) + \nabla p(\rho) = 0, \\ p(\rho) = \omega_\rho(\rho)\rho - \omega(\rho). \end{cases} \tag{13}$$

By taking variation of the dissipation (MDP) (here we assume no-slip boundary conditions: both velocity and its variation vanish at the boundary), one gets

$$L_{\mathbf{x}-}^2 \frac{\delta\mathcal{D}}{\delta_\Omega \mathbf{x}_t} = \frac{\delta\mathcal{D}}{\delta_\Omega \mathbf{u}} = -\eta\Delta\mathbf{u} - \left(\zeta + \frac{1}{3}\eta\right)\nabla\left[\nabla \cdot \mathbf{u}\right].$$

Combining all this into the force balance (4) with MDP yields the compressible Navier-Stokes equations [76]:

$$\begin{cases} \rho_t + \nabla \cdot (\rho\mathbf{u}) = 0, \\ \rho\left(\mathbf{u}_t + (\mathbf{u} \cdot \nabla)\mathbf{u}\right) + \nabla p(\rho) = \eta\Delta\mathbf{u} + \left(\zeta + \frac{1}{3}\eta\right)\nabla\left[\nabla \cdot \mathbf{u}\right], \\ p(\rho) = \omega_\rho(\rho)\rho - \omega(\rho). \end{cases} \tag{14}$$

Remark 7. The flow with pressure depending solely on density is sometimes called barotropic [36]. The choice of function $\omega(\rho)$ results in different specific equations of states for the pressure $p(\rho)$ as follows:

1. Taking the free energy density $\omega(\rho) = a\rho^\gamma$, one can formally obtain the model for isentropic flow of ideal gas with pressure $p = a(\gamma - 1)\rho^\gamma$.
2. In the classical example of isothermal flow of ideal gas, when internal energy does not depend on density (and thus does not affect the dynamics of isothermal flow), the free energy density contains only the contribution of Gibbs entropy $\omega(\rho) = a\rho\ln\rho$, which yields the linear in ρ Boyle's law for pressure $p = a\rho$ [36].

We have derived several important equations in fluid mechanics from LAP and MDP with local mass conservation laws.

3.3   Elasticity and Viscoelasticity

Next under consideration are the models for elastic solids. In elasticity modeling, free energy density depends on the full deformation gradient F [59], not just the determinant (as that for Navier-Stokes energy for the fluids, $W(F) = \omega\left(\frac{\rho_0}{\det F}\right)\det F$). Consequently one needs a reference configuration to conveniently articulate the idea of the deformation with respect to some initial state. Hence, it is common to use Lagrangian coordinates in such models. The energy conservation law in Lagrangian coordinates of a conventional elastic solid is:

$$\frac{d}{dt}\int_\Omega \left(\frac{\rho_0(\mathbf{X})|\mathbf{x}_t|^2}{2} + W(F)\right)d\mathbf{X} = 0, \quad F(\mathbf{X},t) = \frac{\partial\mathbf{x}(X,t)}{\partial\mathbf{X}}. \tag{15}$$

It is clear that one can take $\mathcal{K} = \int_\Omega \frac{\rho_0(\mathbf{X})|\mathbf{x}_t|^2}{2}d\mathbf{X}$, $\mathcal{F} = \int_\Omega W(F)\,d\mathbf{X}$, $\mathcal{D} = 0$ in the energetic variational framework.

The Least Action Principle, the variation with respect to $\mathbf{x}(\mathbf{X},t)$, results in the following force terms:

$$L^2_{\mathbf{X},t-}\frac{\delta\int_0^T \mathcal{K}dt}{\delta_\Omega\mathbf{x}} = -\rho_0(\mathbf{X})\mathbf{x}_{tt}(\mathbf{X},t), \tag{16}$$

$$L^2_{\mathbf{X},t-}\frac{\delta\int_0^T \mathcal{F}dt}{\delta_\Omega\mathbf{x}} = -\nabla_\mathbf{X}\cdot W_F(F). \tag{17}$$

Here $W_F(F) = \left(\frac{\partial W(F)}{\partial F_{ij}}\right)_{ij}$ and $\nabla_\mathbf{X}\cdot M = \left(\sum_j \frac{\partial}{\partial X_j}M_{ij}\right)_i$ for a tensor field M. Hence, the force balance (3) yields the elasticity equation (usually as a hyperbolic type wave equation):

$$\rho_0(\mathbf{X})\mathbf{x}_{tt}(\mathbf{X},t) = \nabla_\mathbf{X}\cdot W_F(F), \tag{18}$$

where W_F is called Piola-Kirchhoff tensor and represents elastic stress in the Lagrangian frame of reference [59, 119].

In the case of linear isotropic elasticity, $W(F) = \frac{1}{2}\lambda\left(|F|^2 - 3\right) = \frac{1}{2}\lambda\left(\text{tr}\left(FF^T\right) - 3\right)$, one gets $W_F = \lambda F = \lambda\nabla_\mathbf{X}\mathbf{x}$, which yields the linear elasticity equation (wave equation):

$$\rho_0\mathbf{x}_{tt} = \lambda\Delta\mathbf{x},$$

where $\lambda > 0$ is the Hookean constant and constant 3 is subtracted to null the energy of the nondeformed material. Here and hereafter Δ denotes the Laplace operator, i.e., $\Delta = \nabla\cdot\nabla$. This model is closely related to neo-Hookean materials, where free energy may also depend on $\det F$ [33]. In [59] free energy density for linear

elastodynamics depends on E, symmetric part of displacement gradient, related to deformation gradient F by $E = \frac{1}{2}\left(F + F^T\right) - I$.

Remark 8. In case of incompressible elasticity , in order to enforce the nonlinear constraint $\det F = 1$, we are tempted to consider the variation of action integral under volume preserving diffeomorphism $\mathbf{x}^\varepsilon$, i.e., $\det \frac{d\mathbf{x}^\varepsilon}{d\mathbf{X}} = 1$. However, it is more convenient to introduce Lagrange multiplier φ and consider variation of $\mathcal{I}(\mathbf{x})$ under no constraint of variation $\mathbf{x}^\varepsilon$, i.e., $\mathbf{x}^0 = \mathbf{x}$, $\frac{d\mathbf{x}^\varepsilon}{d\varepsilon}\big|_{\varepsilon=0} = \delta\mathbf{x}$. Then the variation of

$$\mathcal{I}(\mathbf{x}) = \int_0^T \left[\mathcal{K} - \mathcal{F} - \int \varphi(\mathbf{X}, t) \left(\det \frac{\partial \mathbf{x}}{\partial \mathbf{X}} - 1 \right) d\mathbf{X} \right] dt$$

yields the following incompressible elasticity equation:

$$\begin{cases} \rho_0(\mathbf{X}) \mathbf{x}_{tt}(\mathbf{X}, t) = \nabla_{\mathbf{X}} \cdot \left(W_F(F) + \varphi F^{-T} \right), \\ \det F = 1, \end{cases} \tag{19}$$

where $F^{-T} = (F^{-1})^T$. Note that even for linear isotropic elasticity with Piola-Kirchhoff tensor $W_F = \lambda F$, this equation still has a nonlinear term and the nonlinear constraint.

3.3.1 Eulerian Description of Elasticity

One can also express the elasticity system in Eulerian coordinates . For this one needs to use the deformation tensor in Eulerian coordinates $\tilde{F}(\mathbf{x}(\mathbf{X}, t), t) = F(\mathbf{X}, t)$. Then after coordinate change, the energy law (15) would take form

$$\frac{d}{dt} \int_\Omega \left(\frac{\rho |\mathbf{u}|^2}{2} + \frac{1}{\det \tilde{F}} W(\tilde{F}) \right) d\mathbf{x} = 0.$$

This energy law has to be considered together with mass conservation (11) and kinematic relation for deformation tensor (8), which are consequential from coordinate change. Thus here the kinetic energy is $\mathcal{K} = \int_\Omega \frac{\rho |\mathbf{u}|^2}{2} d\mathbf{x}$, and the free energy is $\mathcal{F} = \int \frac{W(\tilde{F})}{\det \tilde{F}} d\mathbf{X}$. The system is conservative, so there is no dissipation.

Variation of the kinetic energy goes exactly the same as in Sect. 3.2, so

$$L^2_{\mathbf{x},t} - \frac{\delta \int_0^T \mathcal{K} dt}{\delta_\Omega \mathbf{x}} = -\rho \left(\mathbf{u}_t + (\mathbf{u} \cdot \nabla) \mathbf{u} \right).$$

Similarly, for the free energy, we get

$$\delta \int_0^T \mathcal{F} dt = \delta \int_0^T \int W(F) \, d\mathbf{X} dt = \int_0^T \int W_F(F) : \frac{\partial \delta \mathbf{x}}{\partial \mathbf{X}} d\mathbf{X} dt$$
$$= \int_0^T \int \left(W_F(\tilde{F}) \tilde{F}^T : \nabla_{\mathbf{x}} \delta \mathbf{x} \right) \frac{1}{\det \tilde{F}} d\mathbf{x} dt$$
$$= \int_0^T \int \left[-\nabla_{\mathbf{x}} \cdot \left(\frac{W_F(\tilde{F})\tilde{F}^T}{\det \tilde{F}} \right) \right] \cdot \delta \mathbf{x} \, d\mathbf{x} dt = \left\langle -\nabla_{\mathbf{x}} \cdot \left(\frac{W_F(\tilde{F})\tilde{F}^T}{\det \tilde{F}} \right), \delta \mathbf{x} \right\rangle_{L^2_{\mathbf{x},t}}.$$

Hence, the conservative force resulting from this free energy is

$$L^2_{\mathbf{x},t-} \frac{\delta \int_0^T \mathcal{F} dt}{\delta \mathbf{x}} = -\nabla_{\mathbf{x}} \cdot \left(\frac{W_F(\tilde{F}) \tilde{F}^T}{\det \tilde{F}} \right).$$

Writing force balance (3) together with kinematic assumptions (8) and (11), one obtains the following system:

$$\begin{cases} \rho \left(\mathbf{u}_t + (\mathbf{u} \cdot \nabla) \mathbf{u} \right) = \nabla \cdot \left(\frac{W_F(\tilde{F})\tilde{F}^T}{\det \tilde{F}} \right), \\ \tilde{F}_t + (\mathbf{u} \cdot \nabla_{\mathbf{x}}) \tilde{F} = (\nabla_{\mathbf{x}} \mathbf{u}) \tilde{F}, \\ \rho_t + \nabla \cdot (\rho \mathbf{u}) = 0. \end{cases} \tag{20}$$

The term $\frac{W_F(\tilde{F})\tilde{F}^T}{\det \tilde{F}}$ is a Cauchy stress for this system [59, 119]. For the case of linear isotropic elasticity with $W_F = F$ and incompressibility condition $\det F = 1$, it reduces to the left Cauchy-Green tensor $B = FF^T$ [119].

Remark 9. For incompressible viscoelasticity system, one may use the kinetic energy in Eulerian coordinates as $\mathcal{K} = \int_\Omega \frac{\rho |\mathbf{u}|^2}{2} d\mathbf{x}$. The elasticity requires the free energy to depend on the deformation $\tilde{F}$, so $\mathcal{F} = \int_\Omega W(\tilde{F}) \, d\mathbf{x}$. The entropy production (the dissipation) is that from viscosity $\mathcal{D} = \int_\Omega \eta \left| \frac{\nabla u + (\nabla u)^2}{2} \right|^2 d\mathbf{x}$. Again, the incompressibility condition $\det F = 1$ in Lagrangian coordinates is transformed into $\nabla \cdot \mathbf{u} = 0$ in Eulerian coordinates (see Remark 5). The total energy dissipation law takes the form:

$$\frac{d}{dt} \int \left(\frac{\rho |\mathbf{u}|^2}{2} + W(\tilde{F}) \right) d\mathbf{x} = - \int 2\eta \left| \frac{\nabla \mathbf{u} + (\nabla \mathbf{u})^T}{2} \right|^2 d\mathbf{x}. \tag{21}$$

Combining results from Remark 8 and derivation of the system (20) yields $L^2_{\mathbf{x},t-} \frac{\delta \int_0^T \mathcal{K} dt}{\delta \Omega \mathbf{x}} = -\rho \left(\mathbf{u}_t + (\mathbf{u} \cdot \nabla) \mathbf{u} \right)$, $L^2_{\mathbf{x},t-} \frac{\delta \int_0^T \mathcal{F} dt}{\delta \Omega \mathbf{x}} = -\nabla \cdot \left[W_F(\tilde{F}) \tilde{F}^T \right]$, variation of dissipation gives $L^2_{\mathbf{x}-} \frac{\delta \mathcal{D}}{\delta \mathbf{x}_t} = -\eta \Delta \mathbf{u}$, and Lagrange multiplier accounting for incompressibility adds the pressure term ∇p to the force balance because $\delta \mathbf{x}$ should

be restricted as $\nabla \cdot \delta \mathbf{x} = 0$ (as similar to the Remark 5, $\delta \left(\det \frac{\partial \mathbf{x}}{\partial \mathbf{X}} \right) = \nabla \cdot \delta \mathbf{x}$). Hence, the system for incompressible viscoelasticity may be written as follows [84, 91]:

$$
\begin{cases}
\rho \left(\mathbf{u}_t + (\mathbf{u} \cdot \nabla) \mathbf{u} \right) + \nabla p = \nabla \cdot \left(W_F \left(\tilde{F} \right) \tilde{F}^T \right) + \eta \Delta \mathbf{u}, \\
\nabla \cdot \mathbf{u} = 0, \\
\tilde{F}_t + (\mathbf{u} \cdot \nabla_{\mathbf{x}}) \tilde{F} = (\nabla_{\mathbf{x}} \mathbf{u}) \tilde{F}, \\
\rho_t + \nabla \cdot (\rho \mathbf{u}) = 0.
\end{cases}
\tag{22}
$$

## 3.4 Other Approaches to Elastic Fluids

Macroscopic elastic fluids can be realized from many different mechanisms [97], such as those in micro-macro model for polymeric fluid [14, 44] and liquid crystal materials [127].

3.4.1 Micro-Macro Model for Polymeric Fluids

Although the macroscopic continuum mechanics approach dominated the development of rheology in the past, details of the fluid microstructures are often not explicitly taken into account. The hydrodynamical and rheological properties of complex fluids depend intimately on their molecular conformation and configurations [63, 120]. The pure macroscopic descriptions are often not adequate and sufficient to capture the multiscale-multiphysics properties of the materials [14]. The micro-macro or kinetic theory provides an effective "vehicle" to deliver the microscopic information needed in the macroscopic momentum transport [12, 15, 44, 112].

Here the polymeric fluids are used as an example to demonstrate such micro-macro approaches [15, 44]. The micromechanical models for polymeric liquids usually consist of beads joined by springs or rods [84] (see Fig. 3). In the simplest case, a molecule configuration can be described by its end-to-end vector $\mathbf{q}$. Taking

Fig. 3 A schematic illustration of a physical continuum Ω_x and configuration space $\mathbb{R}^3_q$
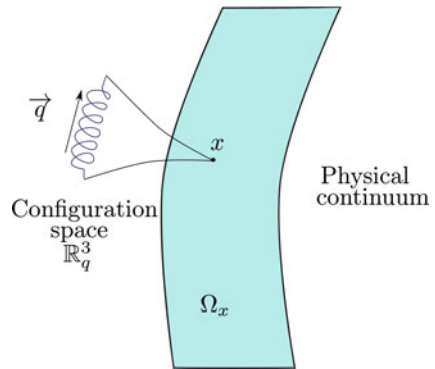
into account the elastic effect together with the thermofluctuation, the probability distribution function [6] $f(\mathbf{x}, \mathbf{q}, t)$ of molecular orientation $\mathbf{q}$ should satisfy the conservation law

$$f_t + \nabla_{\mathbf{x}} \cdot (\mathbf{u} f) + \nabla_{\mathbf{q}} \cdot (\mathbf{V} f) = 0,$$

where $\mathbf{u}(\mathbf{x}, t)$ is macroscopic background velocity and $\mathbf{V}(\mathbf{x}, \mathbf{q}, t)$ is microscopic velocity in the configuration space. For simplicity one may consider the situations when $\nabla \cdot \mathbf{u} = 0$, the macroscopic flow field being incompressible. For each microscopic $\mathbf{q}$, $\Psi(\mathbf{q})$ is the spring energy, which is typically radially symmetric, i.e., depending only on $|\mathbf{q}|$. Then the free energy includes both the entropy and internal energy terms averaged (integrated): $\iint \left(\gamma^2 f \ln f + \Psi f \right) d\mathbf{q} d\mathbf{x}$.

Remark 10. Consider the probability distribution function (PDF) $f(\mathbf{q}, t)$ satisfying the conservation law $f_t + \nabla_{\mathbf{q}} \cdot (\mathbf{V} f) = 0$. Then performing the variation of the energy dissipation law $\frac{d}{dt} \int_{\mathbb{R}^3_q} \left(\gamma^2 f \ln f + \Psi f \right) d\mathbf{q} = -\int_{\mathbb{R}^3_q} \frac{1}{D} f |\mathbf{V}|^2 d\mathbf{q}$ with respect to the flow map generated by $\mathbf{V}$, i.e., $\partial_t \mathbf{q}(\mathbf{Q}, t) = \mathbf{V}(\mathbf{q}(\mathbf{Q}, t), t)$, one gets the convection-diffusion (the Fokker-Planck) equation $f_t = D \nabla_{\mathbf{q}} \cdot \left(\gamma^2 \nabla_{\mathbf{q}} f + f \nabla_{\mathbf{q}} \Psi \right)$. This equation may be obtained as in Sect. 3.2 by setting $\mathcal{F} = \int_{\mathbb{R}^3_q} \left(\gamma^2 f \ln f + \Psi f \right) d\mathbf{q}$ and $\mathcal{D} = \frac{1}{2D} \int_{\mathbb{R}^3_q} f |\mathbf{V}|^2 d\mathbf{q}$. Indeed, the conservation law with the force balance $L^2_{\mathbf{q},t} - \frac{\delta \int_0^T \mathcal{F} dt}{\delta \mathbf{q}} + L^2_{\mathbf{q}-} \frac{\delta \mathcal{D}}{\delta \mathbf{V}} = 0$ yields the desired Fokker-Planck equation. See Sect. 3.5 for similar derivation.

Using the proposed free energy, the energy dissipation law may be postulated as:

$$\frac{d}{dt} \int_{\Omega} \left[\frac{1}{2} \rho |\mathbf{u}|^2 + \lambda \int_{\mathbb{R}^3_q} \left(\gamma^2 f \ln f + \Psi f \right) d\mathbf{q} \right] d\mathbf{x}$$

$$= -\int_{\Omega} \left[2\eta \left| \frac{\nabla_{\mathbf{x}} \mathbf{u} + (\nabla_{\mathbf{x}} \mathbf{u})^T}{2} \right|^2 + \int_{\mathbb{R}^3_q} \frac{\lambda}{D} f |\mathbf{V} - (\nabla_{\mathbf{x}} \mathbf{u}) \mathbf{q}|^2 d\mathbf{q} \right] d\mathbf{x},$$

where kinetic energy is $\mathcal{K} = \int_{\Omega} \frac{1}{2} \rho |\mathbf{u}|^2 d\mathbf{x}$, Helmholtz free energy takes the form of $\mathcal{F} = \lambda \int_{\Omega} \int_{\mathbb{R}^3_q} \left(\gamma^2 f \ln f + \Psi f \right) d\mathbf{q} d\mathbf{x}$, and the energy dissipation functional is equal to $\mathcal{D} = \int_{\Omega} \left[\eta \left| \frac{\nabla_{\mathbf{x}} \mathbf{u} + (\nabla_{\mathbf{x}} \mathbf{u})^T}{2} \right|^2 + \int_{\mathbb{R}^3_q} \frac{\lambda}{2D} f |\mathbf{V} - (\nabla_{\mathbf{x}} \mathbf{u}) \mathbf{q}|^2 d\mathbf{q} \right] d\mathbf{x}$. Here the term $(\nabla_{\mathbf{x}} \mathbf{u}) \mathbf{q}$ accounts for the deformations on microscopic level due to the macroscopic flow. The dissipation on the microlevel is due to relative friction of the particles to the macroscopic flow field. It comes from the configuration space part of convective derivative with configuration space obeying Cauchy-Born rule $\mathbf{q} = F\mathbf{Q}$ and $\mathbf{Q}$ being initial (Lagrangian) configuration. It captures the effect of the macroscopic flow field on the microscopic configurations. Taking full material derivative, one gets:

$$\frac{d}{dt} f\left(\mathbf{x}\left(\mathbf{X}, t\right), F\left(\mathbf{X}, t\right)\mathbf{Q}, t\right) = f_t + \left(\mathbf{u} \cdot \nabla_{\mathbf{x}}\right) f + \left(\left(\nabla_{\mathbf{x}}\mathbf{u}\right)\mathbf{q}\right) \cdot \nabla_{\mathbf{q}} f$$

$$= f_t + \left(\mathbf{u} \cdot \nabla_{\mathbf{x}}\right) f + \nabla_{\mathbf{q}} \cdot \left(\left(\nabla_{\mathbf{x}}\mathbf{u}\right)\mathbf{q} f\right).$$

Note that $\mathbf{q_t}$ in Eulerian coordinates equals $\left(\nabla_{\mathbf{x}}\mathbf{u}\right)\mathbf{q}$. So $\nabla_{\mathbf{q}} \cdot \left(\nabla_{\mathbf{x}}\mathbf{u}\right)\mathbf{q} = \nabla_{\mathbf{x}} \cdot \mathbf{u} = 0$.

To apply the energetic variational approach in this case, it is important to introduce the "separation of scales." It means that on macroscopic level (dynamics of the flow given by $\mathbf{u}$), configuration space follows the flow, i.e., satisfies Cauchy-Born rule $\mathbf{q} = F\mathbf{Q}$ and consequently $\mathbf{V} = \left(\nabla_{\mathbf{x}}\mathbf{u}\right)\mathbf{q}$, while on microscopic level (dynamics of micro-variable f), we treat $\mathbf{q}$ and $\mathbf{V}$ as being independent from $\mathbf{x}$. Thus, on macroscopic level, the free energy written in Lagrangian coordinates $(\mathbf{X}, \mathbf{Q})$ will take the form

$$\mathcal{F} = \lambda \int_{\Omega} \int_{\mathbb{R}^3_q} \left(\gamma^2 f_0\left(\mathbf{X}, \mathbf{Q}\right) \ln f_0\left(\mathbf{X}, \mathbf{Q}\right) + \Psi\left(F\mathbf{Q}\right) f_0\left(\mathbf{X}, \mathbf{Q}\right)\right) d\mathbf{Q} d\mathbf{X}.$$

On microscopic level, we define the flow map in the configuration space $\partial_t \mathbf{q}(\mathbf{x}, \mathbf{Q}, t) = \mathbf{V}(\mathbf{x}, \mathbf{q}(\mathbf{x}, \mathbf{Q}, t), t)$ independently for each $\mathbf{x}$, so the free energy in Lagrangian coordinates will take the form

$$\mathcal{F} = \lambda \int_{\Omega} \int_{\mathbb{R}^3_q} \left(\gamma^2 f_0\left(\mathbf{x}, \mathbf{Q}\right) \ln \frac{f_0\left(\mathbf{x}, \mathbf{Q}\right)}{\det \frac{\partial \mathbf{q}}{\partial \mathbf{Q}}} + \Psi\left(\mathbf{q}\right) f_0\left(\mathbf{x}, \mathbf{Q}\right)\right) d\mathbf{Q} d\mathbf{x}.$$

Performing the variation on macro- and microlevel separately results into the system which includes the kinematic constraints (conservation of mass, incompressibility), as well as force balance laws in both microscopic and macroscopic spaces [84]:

$$\begin{cases} \rho_t + \nabla_{\mathbf{x}} \cdot \left(\rho\mathbf{u}\right) = 0, \\ \rho\left(\mathbf{u}_t + \left(\mathbf{u} \cdot \nabla_{\mathbf{x}}\right)\mathbf{u}\right) + \nabla_{\mathbf{x}} p = \nabla_{\mathbf{x}} \cdot \sigma, \\ \sigma = \eta\left(\nabla_{\mathbf{x}}\mathbf{u} + \left(\nabla_{\mathbf{x}}\mathbf{u}\right)^T\right) - \lambda \int_{\mathbb{R}^3_q} \left(\nabla_{\mathbf{q}}\Psi \otimes \mathbf{q}\right) f d\mathbf{q}, \\ \nabla_{\mathbf{x}} \cdot \mathbf{u} = 0, \\ f_t + \mathbf{u} \cdot \nabla_{\mathbf{x}} f + \nabla_{\mathbf{q}} \cdot \left(\left(\nabla_{\mathbf{x}}\mathbf{u}\right)\mathbf{q} f\right) = D\nabla_{\mathbf{q}} \cdot \left[\gamma^2 \nabla_{\mathbf{q}} f + f \nabla_{\mathbf{q}}\Psi\right]. \end{cases} \tag{23}$$

Notation. *For vectors $\mathbf{a}$ and $\mathbf{b}$, the product $\mathbf{a} \otimes \mathbf{b}$ is the matrix with an element $\left(\mathbf{a} \otimes \mathbf{b}\right)_{ij} = a_i b_j$.*

The elastic stress $M = \int_{\mathbb{R}^3_q} \left(\nabla_{\mathbf{q}}\Psi \otimes \mathbf{q}\right) f d\mathbf{q}$ incorporates the effects of the microscopic configurations into the macroscopic flow by averaging (integrating) in $\mathbf{q}$. In the simplest Hookean spring case, $\Psi = \frac{1}{2}|\mathbf{q}|^2$, if one takes the second moment of f, which is the elastic stress M, as a dependent variable, the system is closed in M, and the well-known Oldroyd-B equations constitutive will be recovered, which has been extensively studied [30, 35, 51, 57, 58, 85]. In general, one may hope that the closure equations will help to solve for approximate f. However,

since the energy law becomes inadequate to provide any closed system for M after this momentum closure procedure, the well-posedness of both the original problem and the closure problem is still not complete except for the local existence [7, 107]. In [84], the well-posedness of the dumbbell system in the near-equilibrium situations was investigated.

It was noticed that the commonly used methods for treating the transport equations, such as the velocity average method [41–43], cannot be (directly) applied here. We observe that the left-hand side of the energy law forbids the presence of the concentration of the singularities when passed to the limits [43, 48]. It is the oscillation of f that needs to be controlled, and new analytical tools have to be developed for these multiscaled transport-parabolic systems.

For more general cases, such as the Finite Extensible Nonlinear Elasticity (FENE) models, there are no finite moment closure systems. Hence, it is important to develop a method to treat such a multiscale system. See [64–66] and their references for specific closure methods developed for FENE systems.

Nematic Liquid Crystals

Liquid crystals and liquid-crystalline polymers constitute a class of complex fluids with anisotropic viscoelastic features due to the orientation of the molecules and their configurations [38]. Not only such materials have seen many applications, the relatively well-developed theories also give the models for other complex fluids.

Let the orientation of particles in nematic liquid crystal be given by the *normed director* $\mathbf{d}(\mathbf{x}, t)$. One can derive the (simplified) Ericksen-Leslie system [78] for small molecule nematic liquid crystal flows by considering the energy dissipation law [82, modified viscous dissipation]:

$$\frac{d}{dt} \int_\Omega \left[\frac{1}{2}\rho \,|\mathbf{u}|^2 + \frac{\lambda}{2}|\nabla\mathbf{d}|^2 + \lambda G(\mathbf{d}) \right] d\mathbf{x}$$
$$= -\int_\Omega \left[2\eta \left| \frac{\nabla\mathbf{u} + (\nabla\mathbf{u})^T}{2} \right|^2 + \frac{\lambda}{\gamma}|\mathbf{d}_t + (\mathbf{u}\cdot\nabla)\mathbf{d}|^2 \right] d\mathbf{x}.$$

The last term in the dissipation $|\mathbf{d}_t + (\mathbf{u}\cdot\nabla)\mathbf{d}|^2$ postulates kinematic assumption on the transport of the director $\mathbf{d}$. For the treatment of more general kinematic assumptions, see [115, 132] and their references.

The competition between kinetic and elastic energy produces the specific properties of the system, such as the existence, stability, and regularity of the hydrostatic configurations [83]. The elastic energy determines the microstructure formation, as well as the defect configurations, and at the same time interacts with the fluid [26, 27, 82, 86]. Such energy laws are important for designing the accurate numerical algorithms [45, 90, 92], especially when the solutions involve singularities.

Using the energetic variational approaches, that is, taking independent variations with respect to the flow map generated by incompressible macroscopic velocity $\mathbf{u}$ and with respect to microscopic director $\mathbf{d}$, one can obtain the following Ericksen-Leslie system:

$$
\begin{cases}
\rho \left(\mathbf{u}_t + (\mathbf{u} \cdot \nabla) \mathbf{u} \right) + \nabla p = \nabla \cdot \sigma, \\
\sigma = \eta \left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T \right) - \lambda (\nabla \mathbf{d} \odot \nabla \mathbf{d}), \\
\mathbf{d}_t + (\mathbf{u} \cdot \nabla) \mathbf{d} = \gamma (\Delta \mathbf{d} - G'(\mathbf{d})), \\
\nabla \cdot \mathbf{u} = 0,
\end{cases}
\tag{24}
$$

where the induced elastic stress $(\nabla \mathbf{d} \odot \nabla \mathbf{d})_{ij} = \sum_{k=1}^{n} (\nabla_i d_k)(\nabla_j d_k)$. In [132], the authors employed the energetic variational derivation of the system for more general elastic energy and energy dissipation functionals.

In liquid crystal flows, there are topological defects due to the constraints on the order parameter and the prescribed boundary conditions [83]. The dynamics of such defects are also governed by elastic effects coupled with the flow. In many cases, there are also flow-induced defects [28]. Usually the number of such defects is very large. The presence of defects can dramatically change the effective properties of the liquid crystal materials. When the effects of fluctuations are taken into account, the defect configuration can melt, and the defects will lose their positional order. The material becomes a "defect liquid," similar to those studied in superconductivity [70, 79, 80, 126]. One approach involves deriving the regularity of the velocity that is independent of the director field and employing the machinery developed in [70, 79, 81]. The fact that the defects will induce flow (back flow) indicates the close coupling between flow and director orientation in these systems. This makes it difficult to derive the explicit dynamics of defects from the momentum equations. Some partial results in case of the velocity being smoother than the Leray solutions have been achieved [83]. The difficulty lies in the convergence of the elastic stress term. See more details and references in the chapter ▸ "Equations for Viscoelastic Fluids".

3.5 Generalized Diffusions

Diffusion is one of the most familiar and studied systems for more than a hundred years [39, 49, 103]. The conventional description involves the conservation law $f_t = \nabla \cdot J$ and the Fick's law stating that J is proportional to ∇f. In this section, the energetic variational structures for diffusion dynamics of a conserved quantity $f(x, t)$ (may be concentration or probability distribution) are going to be explored.

Diffusion of a conserved quantity $f(x, t)$ can be, above all, viewed as a transport:

$$
f_t + \nabla \cdot (f \mathbf{u}) = 0,
\tag{25}
$$

with the energy dissipation law

$$
\frac{d}{dt} \int \omega(f) \, d\mathbf{x} = - \int f \, |\mathbf{u}|^2 \, d\mathbf{x}.
\tag{26}
$$

In the energetic variational framework outlined in the previous section, this energy law corresponds to the kinetic energy $\mathcal{K} = 0$, the free energy $\mathcal{F} = \int_\Omega \omega(f)\, d\mathbf{x}$ (similar to that of fluid), and the energy dissipation $\mathcal{D} = \frac{1}{2} \int_\Omega f\, |\mathbf{u}|^2\, d\mathbf{x}$, which corresponds to Darcy's law (the friction relative to the resting media) in fluid dynamics. Performing a variation with respect to the flow map $\mathbf{x}(\mathbf{X}, t)$ generated by $\mathbf{u}$ (LAP) yields the following conservative force: $L^2_{\mathbf{x},t-}\frac{\delta \int_0^T \mathcal{F} dt}{\delta \mathbf{x}} = \nabla\left(\omega_f(f)\,f - \omega(f)\right)$. The MDP, variation with respect to $\mathbf{u}$, gives $L^2_{\mathbf{x}-}\frac{\delta \mathcal{D}}{\delta \mathbf{u}} = f\mathbf{u}$, and balance of forces (4) results in:

$$f\mathbf{u} + \nabla\left(\omega_f(f)\,f - \omega(f)\right) = 0,$$

which combined with (25) results in a generalized diffusion equation

$$f_t = \Delta\left[\omega_f(f)\,f - \omega(f)\right]. \tag{27}$$

Remark 11. Different models can be obtained by taking various free energy densities.

1. Taking $\omega(f) = \lambda f \ln f$ gives $\omega_f f - \omega = \lambda f$, which results in the linear diffusion equation:

$$f_t = \lambda \Delta f.$$

2. For more complicated free energy density $\omega(f) = \frac{\lambda}{\gamma-1} f^\gamma$, $\gamma > 1$, when particle interactions are involved, one gets $\omega_f f - \omega = \lambda f^\gamma$, which results in the porous medium equation [10, 122]:

$$f_t = \lambda \Delta f^\gamma.$$

3.5.1 Inhomogeneous Diffusions

For diffusion involving spatial inhomogeneities, one can introduce the corresponding energy law:

$$\frac{d}{dt} \int f \ln(a(\mathbf{x})\,f)\, d\mathbf{x} = -\int \frac{f}{a(\mathbf{x})\,b(\mathbf{x})}\, |\mathbf{u}|^2\, d\mathbf{x}.$$

Then the variation yields the following:

$$L^2_{\mathbf{x},t-}\frac{\delta \int_0^T \mathcal{F} dt}{\delta \mathbf{x}} = \frac{1}{a(\mathbf{x})} f \nabla a(\mathbf{x}) + \nabla f, \quad L^2_{\mathbf{x}-}\frac{\delta \mathcal{D}}{\delta \mathbf{u}} = \frac{f}{a(\mathbf{x})\,b(\mathbf{x})}\mathbf{u}.$$

Hence, balance of forces (4) combined with (25) results in linear diffusion equation with variable coefficients:

$$f_t = \nabla \cdot [b(\mathbf{x}) \nabla (a(\mathbf{x}) f)].$$

Notice that the coefficient $a(\mathbf{x})$ from free energy will affect the equilibrium. In particular, if $a(\mathbf{x})$ is not constant, a constant f will no longer be a solution. The other inhomogeneous term $b(\mathbf{x})$ corresponds to the mobility coefficient, which determines the rate of the dynamics approaching the equilibrium.

Remark 12. If terms $a \cdot b = 1$, the equation takes the form of $f_t = \Delta f + \nabla \cdot [\nabla \ln a(\mathbf{x}) f]$, the usual convection-diffusion equation.

Remark 13. Diffusion equation can be interpreted by the Brownian motion [53]. Consider random process

$$d\mathbf{x} = \mathbf{a}(\mathbf{x}) dt + \sigma(\mathbf{x}) dB,$$

where B is standard Brownian motion. Writing a Taylor expansion of probability distribution function $f(\mathbf{x}, t)$, one may obtain the following PDEs:

(a) Ito calculus provides $f_t + \nabla \cdot (\mathbf{a} f) = \frac{1}{2} \Delta (\sigma^2 f)$,
(b) The derivation using Stratonovich integral yields $f_t + \nabla \cdot (\mathbf{a} f) = \frac{1}{2} \nabla \cdot [\sigma \nabla (\sigma f)]$,
(c) Lastly one can derive PDE with self-adjoint diffusion term $f_t + \nabla \cdot (\mathbf{a} f) = \frac{1}{2} \nabla \cdot [\sigma^2 \nabla f]$.

If following fluctuation-dissipation theorem [39, 74], one restricts the convection coefficient $\mathbf{a} = -\frac{1}{2} \sigma^2 \nabla \psi$ and assumes that f satisfies conservation law (25), the equations above may be obtained from variation of the following energy laws:

(a) $\frac{d}{dt} \int \left[f \ln \left(\frac{1}{2} \sigma^2 f \right) + \psi f \right] d\mathbf{x} = -\int \frac{f}{\sigma^2/2} |\mathbf{u}|^2 d\mathbf{x}$,
(b) $\frac{d}{dt} \int \left[f \ln (\sigma f) + \psi f \right] d\mathbf{x} = -\int \frac{f}{\sigma^2/2} |\mathbf{u}|^2 d\mathbf{x}$,
(c) $\frac{d}{dt} \int \left[f \ln f + \psi f \right] d\mathbf{x} = -\int \frac{f}{\sigma^2/2} |\mathbf{u}|^2 d\mathbf{x}$.

3.5.2 Nonlocal Diffusions

Many systems involve nonlocal interactions between particles. Such effects include Coulomb electric interactions, size effects, Lennard-Jones potential, and other nonlocal relations (see, for instance, [23, 68, 123] and their references).

Consider the energy dissipation law with the nonlocal free energy:

$$\frac{d}{dt} \left[\int \lambda f \ln f \, d\mathbf{x} + \iint H(\mathbf{x} - \mathbf{y}) f(\mathbf{y}) f(\mathbf{x}) \, d\mathbf{y} d\mathbf{x} \right] = -\int \eta(f) |\mathbf{u}|^2 d\mathbf{x},$$

$$(28)$$

where $\lambda f \ln f$ is the entropy and $\iint H (\mathbf{x} - \mathbf{y}) f (\mathbf{y}) f (\mathbf{x}) \, d\mathbf{y} d\mathbf{x}$ is the internal energy in the Helmholtz free energy (with λ being constant). Then balance of forces (4) reads as

$$\eta(f)\mathbf{u} + \lambda \nabla f + \left(\nabla \int H (\mathbf{x} - \mathbf{y}) f (\mathbf{y}) \, d\mathbf{y} \right) f = 0,$$

which in the case $\eta(f) = f$ combined with (25) results in the nonlocal diffusion equation as:

$$f_t = \lambda \Delta f + \nabla \cdot \left(f \nabla \int H (\mathbf{x} - \mathbf{y}) f (\mathbf{y}) \, d\mathbf{y} \right). \tag{29}$$

Remark 14. The transport of charged particles is described by a known Poisson-Nernst-Planck (PNP) system [13, 110, 111, 125, 131, 133, 135]. The dynamics takes account of diffusion and convection as well as electrostatics. The system may be written in terms of n and p – densities of negative and positive ions, respectively. Then the energy dissipation law takes the form [133]

$$\frac{d}{dt} \int \left\{ kT (n \log n + p \log p) + \frac{\varepsilon}{2} |\nabla \phi|^2 \right\} d\mathbf{x}$$
$$= - \int kT \left(\frac{n}{D_n} |\mathbf{u}_n|^2 + \frac{p}{D_p} |\mathbf{u}_p|^2 \right) d\mathbf{x}, \tag{30}$$

where D_n and D_p are diffusion constants and $D_n/(kT)$ and $D_p/(kT)$ are mobility constants. Notice that the free energy has both the electric energy (which is nonlocal, as will be shown below) and the entropy (contributing to the diffusion of charge density). ϕ is the electrostatic potential satisfying the Poisson equation:

$$-\varepsilon \Delta \phi = -z_n e \, n + z_p e \, p,$$

where ε is the dielectric constant and z_n and z_p are valences of the ions. Also each density satisfies the conservation law $n_t + \nabla \cdot [\mathbf{u}_n n] = 0$, $p_t + \nabla \cdot [\mathbf{u}_p p] = 0$. To perform the variation, one should resolve the Poisson equation:

$$\phi = \frac{1}{\varepsilon} \int G (\mathbf{x} - \mathbf{y}) \left(-z_n e \, n + z_p e \, p \right) (\mathbf{y}, t) \, d\mathbf{y},$$

where G is a Green's function [50]. Substituting this to the energy law (30), one gets the dissipation law with the nonlocal electric energy term. After combining the variation with respect to the two independent flow maps generated by $\mathbf{u}_n$ and $\mathbf{u}_p$ with conservation laws for the densities, one gets the PNP system:

$$\begin{cases} n_t = \nabla \cdot \left[D_n \nabla n - z_n e \frac{D_n}{kT} n \nabla \phi \right], \\ p_t = \nabla \cdot \left[D_p \nabla p + z_p e \frac{D_p}{kT} p \nabla \phi \right], \\ -\varepsilon \Delta \phi = -z_n e \, n + z_p e \, p. \end{cases} \tag{31}$$

Remark 15. One may notice that the nonlocal effects can be realized even in the model with only the local free energy but with different dissipation contributing the nonlocal term. To get such an effect, instead of Darcy's type dissipation density $f \, |\mathbf{u}|^2$ in (28), one may consider the entropy production (energy dissipation) taking the form similar to the viscosity in fluid dynamics, i.e.,

$$\mathcal{D} = \frac{1}{2} \int \eta \, |\nabla \mathbf{u}|^2 \, d\mathbf{x}.$$

Then (with $\mathcal{K} = 0$, $\mathcal{F} = \int_\Omega \omega \, (f) \, d\mathbf{x}$) the force balance equation (4) will yield the Poisson equation for $\mathbf{u}$:

$$\nabla p = \eta \Delta \mathbf{u}, \quad p = \omega_f \, (f) \, f - \omega \, (f).$$

Solving for $\mathbf{u}$ in terms of p, one can (formally) get

$$\mathbf{u} = -\frac{1}{\eta} \nabla \int G \, (\mathbf{x} - \mathbf{y}) \, p \, (f) \, (\mathbf{y}, t) \, d\mathbf{y},$$

where G is a Green's function. Substituted to (25), this gives a nonlocal diffusion equation:

$$f_t - \nabla \cdot \left(\frac{f}{\eta} \nabla \int G \, (\mathbf{x} - \mathbf{y}) \, p \, (f) \, (\mathbf{y}, t) \, d\mathbf{y} \right) = 0. \tag{32}$$

This corresponds to $\lambda = 0$, $p = f$, and $H = G/\eta$ in (29) while being derived from totally different physics (energy laws).

4   Complex Fluid Mixtures: Diffusive Interface Models

4.1   Surface Tension and the Sharp Interface Formulation

Interface problems arising in mixtures of different fluids, solids, and gases have attracted attention for more than two centuries. Many surface properties, such as capillarity, are associated with the surface tension through special boundary conditions [72, 73]. The classical approach to this problem usually considers the interface to be a free surface that evolves in time with the fluid velocity [60].

Fig. 4 A schematic illustration of domain Ω with two fluids separated by free interface Γ_t

$$\Omega = \Omega_1 \cup \Omega_2$$
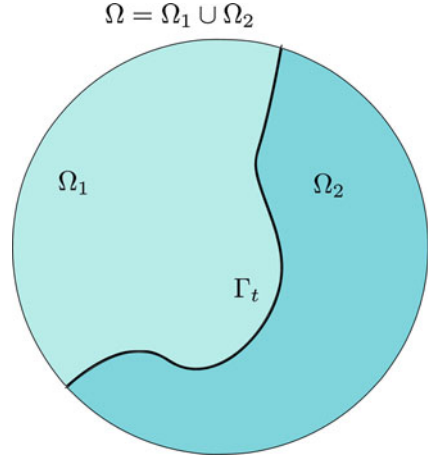
Consider domain Ω with two incompressible fluids occupying subdomains Ω_1 and Ω_2 (see Fig. 4) and $\Gamma_t = \overline{\Omega_1} \cap \overline{\Omega_2}$ free interface between the two fluids. Classical approach to this problem yields incompressible Navier-Stokes equation in each subdomain:

$$\begin{cases} \rho_i \left(\mathbf{u}_t^i + \left(\mathbf{u}^i \cdot \nabla \right) \mathbf{u}^i \right) + \nabla p_i = \eta_i \Delta \mathbf{u}^i, \\ \nabla \cdot \mathbf{u}^i = 0, \end{cases} \quad \text{in } \Omega_i. \tag{33}$$

Define Cauchy stress tensor τ_i by the following relation [119]:

$$\eta_i \Delta \mathbf{u}^i - \nabla p = \nabla \cdot \tau_i \quad \text{with} \quad \tau_i = \eta_i \left(\nabla \mathbf{u}^i + \left(\nabla \mathbf{u}^i \right)^T \right) - p_i I.$$

Then the position of the interface at each individual time is determined by the immiscibility condition

$$\mathbf{u}^i \cdot \nu = V_n \tag{34}$$

and the Young-Laplace stress free (force balance) condition (see, for instance, [9]):

$$[\tau] \cdot \nu = -\sigma H \nu,$$

where $[\tau]$ is the jump of the stress across the interface Γ_t, with ν its normal, H the mean curvature of the surface, and σ the surface tension constant. Also we assume no-slip condition both on the boundary and on the interface

$$\mathbf{u}^i = 0 \text{ on } \partial\Omega, \quad [\mathbf{u}] = 0 \text{ on } \Gamma_t.$$

Since,

$$\int_{\Gamma_t} V_n \cdot [\tau] \cdot \nu \, dS_\mathbf{x} = \int_{\Gamma_t} -\sigma H V_n \cdot \nu \, dS_\mathbf{x} = -\frac{d}{dt} \sigma \, \text{area} \Gamma_t,$$

multiplying first equation in (33) by $\mathbf{u}^i$ and integrating over Ω_i for $i = 1, 2$, one can get the energy dissipation law:

$$\frac{d}{dt}\left[\sum_{i=1,2}\int_{\Omega_i}\frac{1}{2}\rho\left|\mathbf{u}^i\right|d\mathbf{x} + \sigma\ \mathrm{area}\Gamma_t\right] = -\sum_{i=1,2}\int_{\Omega_i}2\eta_i\left|\frac{\nabla\mathbf{u}^i + (\nabla\mathbf{u}^i)^T}{2}\right|^2 d\mathbf{x}.$$

(35)

4.2 Diffusive Interface Approximations (Phase Field Methods)

To regularize the transition between two phases, here the statistical point of view (or phase field approach) is employed, which treats the interface as a continuous, but steep, change of properties (density, viscosity, etc.) of the two fluids. Within a "thin" transition region, the fluid is mixed and has to store certain amount of "mixing energy." Such an approach coincides with the usual phase field models in the theory of phase transition [24, 25, 95, 98, 117, 128]. These models will allow the topological change of the interface [93] and have many advantages when simulating front motions [29]. Recently many researchers have employed the phase field approach for various fluid models [4, 16, 18, 19, 31, 32, 62, 69, 71, 88, 91, 96, 104].

Suppose that the interface Γ_t has thickness $O(\varepsilon)$. Then consider phase field satisfying

$$\varphi(\mathbf{x}) = \begin{cases} 1, & \text{in } \Omega_1 \\ -1, & \text{in } \Omega_2, \end{cases}$$

which takes values in $(-1, 1)$ on the diffusive interface. φ may not necessarily be an obvious physical quantity (like concentration or volume fraction) but just a labeling function representing the smooth transition between phases.

Following [25], here the mixing energy is introduced as a functional of φ to approximate the interface term in the energy (35)

$$\frac{\lambda}{\sigma}\mathcal{W}(\varphi) = \frac{\lambda}{\sigma}\int\frac{1}{2}|\nabla\varphi|^2 + \frac{1}{\varepsilon^2}G(\varphi)\,d\mathbf{x} \approx \mathrm{area}\Gamma_t,$$

(36)

where G is a so-called double-well potential (e.g., $G(\varphi) = \frac{1}{4}(\varphi^2 - 1)^2$), ε is a parameter responsible for the "width" of the interface, and λ/σ depends on $G(\varphi)$ and ε (for given example $\lambda = \frac{3\varepsilon}{2\sqrt{2}}\sigma$, see [134]). The gradient term in this energy is diffusive ("philic," represents weakly nonlocal interactions between the components that prefers complete mixing), while the second term is Ginzburg-Landau potential (repulsion potential, "phobic," prefers total separation of the phases). The competition between the two effects defines the profile of φ across the interface.

Remark 16. The study of the physics of biological membranes of vesicles such as cells and liposomes may involve more complicated forms of surface bending energy. One example of such elastic energy [46] may take the form:

$$E = \int_{\Gamma} k(H - c_0)^2 \, dS, \tag{37}$$

where $H = (k_1 + k_2)/2$ is the mean curvature of the membrane surface, with k_1 and k_2 as the principle curvatures, k is the bending rigidity, and c_0 is the spontaneous curvature that describes the asymmetry effect of the membrane or its environment. The equilibrium configuration of the vesicle membrane is determined by minimizing the above elastic bending energy with prescribed volume and surface area constraints. To approximate this energy by phase field, one can write

$$E_\varepsilon(\varphi) = \frac{3\sqrt{2}k}{16\varepsilon} \int_{\Omega} \left(\varepsilon\Delta\varphi + \left(\frac{1}{\varepsilon}\varphi + c_0\sqrt{2} \right) \left(1 - \varphi^2 \right) \right)^2 \, d\mathbf{x}; \tag{38}$$

the volume of the region enclosed by the membrane will be determined by ($V = (|\Omega| + A(\varphi))/2$): $A(\varphi) = \int_{\Omega} \varphi \, d\mathbf{x}$, and the surface area of the membrane is determined by (up to a constant) $B_\varepsilon(\varphi) = \int_{\Omega} \frac{\varepsilon}{2} |\nabla\varphi|^2 + \frac{1}{4\varepsilon}(\varphi^2 - 1)^2 \, d\mathbf{x}$. The original spontaneous curvature c_0 is defined only on the surface Γ (it may vary on the surface, representing a heterogeneity of the membrane). We extend c_0 to the whole domain Ω in a way that, in a neighborhood of Γ, c_0 is constant in the direction normal to Γ. The equilibrium configuration is obtained by minimizing the above elastic bending energy $E_\varepsilon(\varphi)$ with the constraints that $A(\varphi)$ and $B_\epsilon(\varphi)$ are constants. See [46] for convergence of $E_\varepsilon(\varphi)$ to E as $\varepsilon \to 0$.

More complicated form of elastic bending energy is a part of the Helfrich model, which has been studied extensively in the literature in recent years (see [34,102,113, 114] and additional references in [47]). This is also related to the classical Willmore problem in differential geometry [130].

Now, taking $\mathbf{u}$ to be incompressible background velocity (e.g., volume-averaged [1]), not the velocity of either of fluids, the following kinetic and Helmholtz free energy follows:

$$\mathcal{K} = \int \frac{\rho(\varphi) |\mathbf{u}|^2}{2} d\mathbf{x}, \ \mathcal{F} = \lambda\mathcal{W}(\varphi). \tag{39}$$

In addition, on macroscopic level, it is sensible to impose immiscibility condition (9), which is equivalent to (34). While using this approximation, one can introduce additional microscopic dissipative term for regularization purposes (introducing energy dissipation on the diffusive interface). If one takes microscopic dynamics to be that of gradient flow (and introducing appropriate dissipation $\mathcal{D}$), variation produces Allen-Cahn/Navier-Stokes system, while to get the phase field to

satisfy conservation law, one can introduce "Darcy's like" dissipation (proportional to relative drag) and deduce Cahn-Hilliard/Navier-Stokes system.

4.2.1 Allen-Cahn/Navier-Stokes Systems

Here the following energy dissipation law is considered [67, modified viscous dissipation]:

$$\frac{d}{dt}\left(\mathcal{K} + \mathcal{F}\right) = -\int_{\Omega}\left[2\eta\left(\varphi\right)\left|\frac{\nabla\mathbf{u} + \left(\nabla\mathbf{u}\right)^T}{2}\right|^2 + \frac{1}{\gamma}\left|\varphi_t + \left(\mathbf{u}\cdot\nabla\right)\varphi\right|^2\right]d\mathbf{x},$$

(40)

where $\mathcal{K}$ and $\mathcal{F}$ are taken from (39). There are two quantities of interest in this model: $\mathbf{u}$ and φ, so the variation will be performed for each of them separately.

First, we look at the microscopic dynamics on the interface given by Allen-Cahn equation [3]. It can be seen as gradient flow with convection in microscale variable φ:

$$\varphi_t + \left(\mathbf{u}\cdot\nabla\right)\varphi = -\gamma\left(L_{\mathbf{x},t-}^2\frac{\delta\int_0^T\left(\mathcal{K} + \mathcal{F}\right)dt}{\delta\varphi}\right)$$

To get this equation from energy dissipation law (40) as force balance for variable φ, one may to notice that variation of kinetic energy $\int\frac{1}{2}\rho\left|\mathbf{u}\right|^2 d\mathbf{x}$ gives inertial force only when performed with respect to the flow map generated by $\mathbf{u}$. So performing variation with respect to φ, the total energy $\mathcal{K} + \mathcal{F}$ should be treated altogether as Helmholtz free energy. So the variation goes as

$$\delta_\varphi\int_0^T\mathcal{K} + \mathcal{F}dt = \int_0^T\int_\Omega\left[\frac{\rho'(\varphi)|\mathbf{u}|^2}{2}\delta\varphi + \lambda\left(\nabla\varphi\cdot\nabla\delta\varphi + \frac{1}{\varepsilon^2}G'\left(\varphi\right)\delta\varphi\right)\right]d\mathbf{x}dt$$
$$= \int_0^T\int_\Omega\left[\frac{\rho'(\varphi)|\mathbf{u}|^2}{2} + \lambda\left(-\Delta\varphi + \frac{1}{\varepsilon^2}G'\left(\varphi\right)\right)\right]\delta\varphi d\mathbf{x}dt$$
$$+ \int_0^T\int_{\partial\Omega}\left(\nabla\varphi\cdot\nu\right)\delta\varphi\, dS_\mathbf{x}dt.$$

Notation. *Here we have two quantities of interest: φ and $\mathbf{u}$. So one has to adapt the variational notation to multiple variations of the same functional. Thus, here*

$$\delta_\varphi\int_0^T\mathcal{K}dt = \lim_{h\to 0}\int_0^T\frac{\mathcal{K}\left(\varphi + h\delta\varphi, \mathbf{x}\right) - \mathcal{K}\left(\varphi, \mathbf{x}\right)}{h}dt,$$

$$\delta_\mathbf{x}\int_0^T\mathcal{K}dt = \lim_{h\to 0}\int_0^T\frac{\mathcal{K}\left(\varphi, \mathbf{x} + h\delta\mathbf{x}\right) - \mathcal{K}\left(\varphi, \mathbf{x}\right)}{h}dt,$$

and similarly for other functionals.

To cancel the boundary effects, one would make the boundary term in the variation equal to zero, which results in the boundary condition $\nabla\varphi\cdot\nu = 0$. Then the force

balance (4) can be rewritten as $L^2_{\mathbf{x},t-}\frac{\delta \int_0^T \mathcal{K}dt}{\delta \varphi} + L^2_{\mathbf{x},t-}\frac{\delta \int_0^T \mathcal{F}dt}{\delta \varphi} + L^2_{\mathbf{x}-}\frac{\delta \mathcal{D}}{\delta \varphi_t} = 0$, which reads as follows

$$
\begin{cases}
\frac{\rho'(\varphi)|\mathbf{u}|^2}{2} + \lambda\left[-\Delta\varphi + \frac{1}{\varepsilon^2}G'(\varphi)\right] + \frac{1}{\gamma}(\varphi_t + (\mathbf{u}\cdot\nabla)\varphi) = 0, & \mathbf{x} \in \Omega, \\
\nabla\varphi \cdot \nu = 0, & \mathbf{x} \in \partial\Omega.
\end{cases}
$$

Now, considering macro-scale background flow $\mathbf{u}$ yields the variation with respect to flow map $\mathbf{x}(\mathbf{X}, t)$. When writing macroscopic force balance, to account for "separation of scales," one should consider microscopic variable φ to be transported with the flow, i.e., satisfy Eq. (9), so one has to include only viscous part of dissipation $\mathcal{D}_\eta = \int_\Omega \eta(\varphi)\left|\frac{\nabla\mathbf{u}+(\nabla\mathbf{u})^T}{2}\right|^2 d\mathbf{x}$ in the variation. Performing the variation (subject to the assumption $\det F = 1$ or equivalently $\nabla \cdot \mathbf{u} = 0$) yields

$$
\begin{aligned}
\delta_{\mathbf{x}}\int_0^T \mathcal{K}dt &= \delta_{\mathbf{x}}\int_0^T \int_\Omega \frac{1}{2}\rho(\varphi_0(\mathbf{X}))|\mathbf{x}_t(\mathbf{X}, t)|^2 d\mathbf{X}dt \\
&= \int_0^T \int_\Omega [-\rho(\varphi)(\mathbf{u}_t + (\mathbf{u}\cdot\nabla)\mathbf{u})\cdot\delta\mathbf{x}]\,d\mathbf{x}dt,
\end{aligned}
$$

$$
\begin{aligned}
\delta_{\mathbf{x}}\int_0^T \mathcal{F}dt &= \delta_{\mathbf{x}}\int_0^T \int_\Omega \lambda\left[\frac{1}{2}\left|F^{-1}\nabla_{\mathbf{X}}(\varphi_0)\right|^2 + \frac{1}{\varepsilon^2}G(\varphi_0)\right]d\mathbf{X}dt \\
&= \int_0^T \int_\Omega \lambda[\nabla\cdot(\nabla\varphi\otimes\nabla\varphi)]\cdot\delta\mathbf{x}\,d\mathbf{x}dt \\
&\quad - \int_0^T \int_{\partial\Omega} \lambda(\nabla\varphi\cdot\nu)\nabla\varphi\cdot\delta\mathbf{x}\,dS_{\mathbf{x}}dt,
\end{aligned}
$$

$$
\begin{aligned}
\delta_{\mathbf{u}}\mathcal{D}_\eta &= \int_\Omega \eta\left(\left(\frac{\nabla\mathbf{u}+(\nabla\mathbf{u})^T}{2}\right):\left(\nabla\delta\mathbf{u}+(\nabla\delta\mathbf{u})^T\right)\right)d\mathbf{x} \\
&= \int_\Omega -\nabla\cdot\left[\eta\left(\nabla\mathbf{u}+(\nabla\mathbf{u})^T\right)\right]\cdot\delta\mathbf{u}\,d\mathbf{x} \\
&\quad + \int_{\partial\Omega} \eta\left(\nabla\delta\mathbf{u}+(\nabla\delta\mathbf{u})^T\right):(\delta\mathbf{u}\otimes\nu)\,dS_{\mathbf{x}}.
\end{aligned}
$$

Notation. *For two matrices A and B, the scalar product $A : B = \sum\limits_{i,j} A_{i,j}B_{i,j}$.*

Remark 17. When taking the variation of kinetic energy $\mathcal{K}$, one can perform integration by parts (in t) after changing the coordinates back to Eulerian. Then the variation would result in $L^2_{\mathbf{x},t-}\frac{\delta \int_0^T \mathcal{K}dt}{\delta\mathbf{x}} = -(\rho(\varphi)\mathbf{u})_t - (\mathbf{u}\cdot\nabla)(\rho(\varphi)\mathbf{u})$.

Hence, force balance may be written as $L^2_{\mathbf{x},t-}\frac{\delta \int_0^T \mathcal{K}dt}{\delta\mathbf{x}} = L^2_{\mathbf{x},t-}\frac{\delta \int_0^T \mathcal{F}dt}{\delta\mathbf{x}} + L^2_{\mathbf{x}-}\frac{\delta\mathcal{D}_\eta}{\delta\mathbf{u}}$, which yields

$$
\rho(\varphi)(\mathbf{u}_t + (\mathbf{u}\cdot\nabla)\mathbf{u}) + \nabla p = \nabla\cdot\left[\eta\left(\nabla\mathbf{u}+(\nabla\mathbf{u})^T\right)\right] - \lambda\nabla\cdot(\nabla\varphi\otimes\nabla\varphi), \quad \mathbf{x}\in\Omega,
$$
(41)

and on the boundary, the condition $\mathbf{u} = 0$ is taken, which yields $\delta\mathbf{u} = 0$, so takes care the boundary term.

Altogether this results in the Allen-Cahn/Navier-Stokes system [89]:

$$
\begin{cases}
\varphi_t + (\mathbf{u} \cdot \nabla)\varphi = \gamma\lambda\left[\Delta\varphi - \frac{1}{\varepsilon^2}G'(\varphi)\right] - \frac{\gamma}{2}\rho'(\varphi)|\mathbf{u}|^2, & \mathbf{x} \in \Omega, \\
\rho(\varphi)(\mathbf{u}_t + (\mathbf{u} \cdot \nabla)\mathbf{u}) + \nabla p = \nabla \cdot \left[\eta\left(\nabla\mathbf{u} + (\nabla\mathbf{u})^T\right)\right] \\
\qquad\qquad\qquad\qquad\qquad\qquad - \lambda\nabla \cdot (\nabla\varphi \otimes \nabla\varphi), & \mathbf{x} \in \Omega, \\
\nabla \cdot \mathbf{u} = 0, & \mathbf{x} \in \Omega, \\
\mathbf{u} = 0, \ \nabla\varphi \cdot \nu = 0, & \mathbf{x} \in \partial\Omega.
\end{cases}
\tag{42}
$$

Remark 18. In order to get the system without the $\frac{\gamma}{2}\rho'(\varphi)|\mathbf{u}|^2$ term in the first equation, one can use $\frac{1}{2}\left[\rho(\varphi)(\mathbf{u}_t + (\mathbf{u} \cdot \nabla)\mathbf{u}) + (\rho(\varphi)\mathbf{u})_t + (\mathbf{u} \cdot \nabla)(\rho(\varphi)\mathbf{u})\right]$ as a convective term in the second equation.

4.2.2 Cahn-Hilliard/Navier-Stokes Systems

Now assume that phase field satisfies conservation law:

$$
\varphi_t + \nabla \cdot (\varphi\mathbf{V}) = 0,
\tag{43}
$$

and energy law [21]

$$
\frac{d}{dt}(\mathcal{K} + \mathcal{F}) = -\int_\Omega\left[2\eta(\varphi)\left|\frac{\nabla\mathbf{u} + (\nabla\mathbf{u})^T}{2}\right|^2 + \varphi^2\left\langle M^{-1}(\varphi)(\mathbf{V} - \mathbf{u}), (\mathbf{V} - \mathbf{u})\right\rangle\right]d\mathbf{x}.
\tag{44}
$$

On macro-scale the variation is identical to the gradient flow case so gives Eq. (41). To perform variation on microscopic interfacial scale, one should define flow map $\mathbf{x}_\varphi(\mathbf{X}, t)$ as $\partial_t\mathbf{x}_\varphi = \mathbf{V}$ and $\mathbf{x}_\varphi(\mathbf{X}, 0) = \mathbf{X}$. We treat the macroscopic flow velocity $\mathbf{u}$ is fully independent from $\mathbf{x}_\varphi$. And, as in gradient flow case, kinetic energy $\mathcal{K}$ is treated as a part of free energy. Using (10), one gets

$$
\begin{aligned}
\delta_{\mathbf{x}_\varphi}\int_0^T\mathcal{K}dt &= \delta\int_0^T\int_\Omega\frac{1}{2}\rho\left(\frac{\varphi_0(\mathbf{X})}{\det\frac{\partial\mathbf{x}_\varphi}{\partial\mathbf{X}}}\right)|\mathbf{u}|^2\det\frac{\partial\mathbf{x}_\varphi}{\partial\mathbf{X}}d\mathbf{X}dt \\
&= \int_0^T\int_\Omega\frac{1}{2}\nabla_{\mathbf{x}_\varphi}\left[\rho'(\varphi)\varphi - \rho(\varphi)\right]|\mathbf{u}|^2 \cdot \delta\mathbf{x}_\varphi \, d\mathbf{x}dt \\
&= \int_0^T\int_\Omega\varphi\nabla\left[\frac{1}{2}\rho'(\varphi)|\mathbf{u}|^2\right] \cdot \delta\mathbf{x}_\varphi \, d\mathbf{x}dt,
\end{aligned}
$$

$$
\begin{aligned}
\delta_{\mathbf{x}_\varphi}\int_0^T\mathcal{F}dt &= \delta\int_0^T\int_\Omega\lambda\left[\frac{1}{2}\left|F^{-1}\nabla_{\mathbf{X}}\left(\frac{\varphi_0(\mathbf{X})}{\det\frac{\partial\mathbf{x}_\varphi}{\partial\mathbf{X}}}\right)\right|^2 + \frac{1}{\varepsilon^2}G\left(\frac{\varphi_0(\mathbf{X})}{\det\frac{\partial\mathbf{x}_\varphi}{\partial\mathbf{X}}}\right)\right]d\mathbf{X}dt \\
&= \int_0^T\int_\Omega\lambda\varphi\nabla\left[-\Delta\varphi + \frac{1}{\varepsilon^2}G'(\varphi)\right] \cdot \delta\mathbf{x}_\varphi \, d\mathbf{x}dt \\
&\quad + \int_0^T\int_{\partial\Omega}\lambda\left(-\nabla \cdot (\varphi\delta\mathbf{x}_\varphi)\right)(\nabla\varphi \cdot \nu) \\
&\quad + \lambda\left(\frac{1}{2}|\nabla\varphi|^2 + \varphi\Delta\varphi + \frac{1}{\varepsilon^2}[G(\varphi) - \varphi G'(\varphi)]\right)\left(\delta\mathbf{x}_\varphi \cdot \nu\right) dS_{\mathbf{x}}dt,
\end{aligned}
$$

$$
\delta_{\mathbf{V}}\mathcal{D} = \int_\Omega\varphi^2 M^{-1}(\varphi)(\mathbf{V} - \mathbf{u}) \cdot \delta\mathbf{V} \, d\mathbf{x}.
$$

Thus, the force balance $\varphi^2 M^{-1}(\varphi)(\mathbf{V} - \mathbf{u}) + \varphi \nabla \left[-\lambda \Delta \varphi + \lambda \frac{1}{\varepsilon^2} G'(\varphi) + \frac{1}{2}\rho'(\varphi)|\mathbf{u}|^2 \right] = 0$, combined with (43), leads to Cahn-Hilliard equation

$$\varphi_t + (\mathbf{u} \cdot \nabla)\varphi = \nabla \cdot [M(\varphi)\nabla\mu], \quad \mu = -\lambda \Delta \varphi + \lambda \frac{1}{\varepsilon^2} G'(\varphi) + \frac{1}{2}\rho'(\varphi)|\mathbf{u}|^2 .$$

Force balance on the boundary gives $\nabla \varphi \cdot \nu = 0$, $\mathbf{V} \cdot \nu = 0$ (second condition yields $\delta \mathbf{x}_\varphi \cdot \nu = 0$). Notice that $\mu = L^2_{\mathbf{x},t-} \frac{\delta \int_0^T \mathcal{K} dt}{\delta \varphi} + L^2_{\mathbf{x},t-} \frac{\delta \int_0^T \mathcal{F} dt}{\delta \varphi}$ is the same variational gradient as in Allen-Cahn equation. All combined with boundary conditions leads to Cahn-Hilliard/Navier-Stokes system :

$$
\begin{cases}
\varphi_t + (\mathbf{u} \cdot \nabla)\varphi = \nabla \cdot [M(\varphi)\nabla\mu], & \mathbf{x} \in \Omega, \\
\mu = -\lambda \Delta \varphi + \lambda \frac{1}{\varepsilon^2} G'(\varphi) + \frac{1}{2}\rho'(\varphi)|\mathbf{u}|^2 , & \\
\rho(\varphi)(\mathbf{u}_t + (\mathbf{u} \cdot \nabla)\mathbf{u}) + \nabla p = \nabla \cdot \left[\eta \left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T \right) \right] & \\
\qquad\qquad\qquad\qquad\qquad - \lambda \nabla \cdot (\nabla \varphi \otimes \nabla \varphi), & \mathbf{x} \in \Omega, \\
\nabla \cdot \mathbf{u} = 0, & \mathbf{x} \in \Omega, \\
\mathbf{u} = 0, \ \nabla \varphi \cdot \nu = 0, \ M(\varphi)\nabla\mu \cdot \nu = 0, & \mathbf{x} \in \partial\Omega.
\end{cases}
\tag{45}
$$

Remark 19. For the system (45), the phase field effective velocity $\mathbf{V}$ is defined up to a term $\tilde{\mathbf{V}}$ with $\nabla \cdot \left(\varphi \tilde{\mathbf{V}} \right) = 0$, which results in nonuniqueness of the energy law (44). To eliminate this drawback, one may employ the operator $R\cdot = (-\Delta)^{1/2}\nabla\cdot$ and with $M = 1$ consider the following energy dissipation law:

$$\frac{d}{dt}(\mathcal{K} + \mathcal{F}) = -\int_\Omega \left[2\eta(\varphi) \left| \frac{\nabla \mathbf{u} + (\nabla \mathbf{u})^T}{2} \right|^2 + |R \cdot (\varphi \mathbf{V} - \varphi \mathbf{u})|^2 \right] d\mathbf{x}.$$

Performing the variational procedure on this energy law, one would still get system (45).

Remark 20. To formally derive **conservative Allen-Cahn/Navier-Stokes system**, consider energy law (40) constraint by conservation law (43), which may be rewritten as

$$\frac{d}{dt}(\mathcal{K} + \mathcal{F}) = -\int_\Omega \left[2\eta(\varphi) \left| \frac{\nabla \mathbf{u} + (\nabla \mathbf{u})^T}{2} \right|^2 + \frac{1}{\gamma} |\nabla \cdot (\varphi \mathbf{V} - \varphi \mathbf{u})|^2 \right] d\mathbf{x}.
\tag{46}$$

Once again, macroscopic force balance yields Navier-Stokes equation (41), while microscopic force balance reads as

$$\varphi \nabla \left[-\frac{1}{\gamma} \nabla \cdot (\varphi \mathbf{V} - \varphi \mathbf{u}) - \lambda \Delta \varphi + \lambda \frac{1}{\varepsilon^2} G'(\varphi) + \frac{1}{2} \rho'(\varphi) |\mathbf{u}|^2 \right] = 0,$$

or

$$-\nabla \cdot (\varphi \mathbf{V}) + (\mathbf{u} \cdot \nabla) \varphi = -\gamma \left[-\lambda \Delta \varphi + \lambda \frac{1}{\varepsilon^2} G'(\varphi) + \frac{1}{2} \rho'(\varphi) |\mathbf{u}|^2 \right] + C.$$

Integrating this equation over Ω and using boundary conditions $\mathbf{u} = 0$, $\nabla \varphi \cdot \nu = 0$, $\mathbf{V} \cdot \nu = 0$ yield $C = \frac{1}{|\Omega|} \gamma \int_\Omega \lambda \frac{1}{\varepsilon^2} G'(\varphi) + \frac{1}{2} \rho'(\varphi) |\mathbf{u}|^2 \, d\mathbf{x}$, which altogether give nonlocal Allen-Cahn/Navier-Stokes system:

$$\begin{cases} \varphi_t + (\mathbf{u} \cdot \nabla) \varphi = \gamma \left[-\mu + \frac{1}{|\Omega|} \int_\Omega \mu \, d\mathbf{x} \right], & \mathbf{x} \in \Omega, \\ \mu = -\lambda \Delta \varphi + \lambda \frac{1}{\varepsilon^2} G'(\varphi) + \frac{1}{2} \rho'(\varphi) |\mathbf{u}|^2, & \\ \rho(\varphi) (\mathbf{u}_t + (\mathbf{u} \cdot \nabla) \mathbf{u}) + \nabla p = \nabla \cdot \left[\eta \left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T \right) \right] & \\ \qquad\qquad -\lambda \nabla \cdot (\nabla \varphi \otimes \nabla \varphi), & \mathbf{x} \in \Omega, \\ \nabla \cdot \mathbf{u} = 0, & \mathbf{x} \in \Omega, \\ \mathbf{u} = 0, \ \nabla \varphi \cdot \nu = 0, & \mathbf{x} \in \partial\Omega. \end{cases} \tag{47}$$

4.3 Boundary Conditions in the Diffusive Interface Models

Authors of [105] have shown that the model with energy dissipation at the solid boundary surface better matches molecular dynamics experiments and avoids discrepancy of the contact line dynamics. More precisely, standard boundary conditions do not allow contact line to move along the boundary, while molecular dynamics experiments show that near-complete slip occurs in vicinity of contact line near the boundary.

Hence, one may consider the following expression for energy dissipation (including bulk terms already mentioned above):

$$\mathcal{D} = \frac{1}{2} \int_\Omega \left(2\eta(\varphi) \left| \frac{\nabla \mathbf{u} + (\nabla \mathbf{u})^T}{2} \right|^2 + \varphi^2 \langle M^{-1}(\varphi) (\mathbf{V} - \mathbf{u}), (\mathbf{V} - \mathbf{u}) \rangle \right) d\mathbf{x}$$
$$+ \frac{1}{2} \int_{\partial\Omega} \left(\beta |\mathbf{u}_\tau|^2 + \frac{3\varepsilon}{2\sqrt{2}} \frac{\sigma}{\gamma} |\varphi_t + (\mathbf{u}_\tau \cdot \nabla_\tau) \varphi|^2 \right) dS_x,$$

where subscript τ denotes components tangential to the boundary (e.g., $\mathbf{u}_\tau = \mathbf{u} - (\mathbf{u} \cdot \nu) \nu$). The force balance after combining LAP and MDP results into the dynamic boundary conditions on φ and generalized Navier boundary conditions on $\mathbf{u}$:

$$\begin{cases} \varphi_t + (\mathbf{u}_\tau \cdot \nabla_\tau)\,\varphi + \gamma \partial_\nu \varphi = 0, \quad \langle M\,(\varphi)\,\nabla\mu,\,\nu \rangle = 0, \\ \beta\,(\mathbf{u}_\tau) + \eta\,(\varphi)\,\partial_\nu\,(\mathbf{u}_\tau) - \sigma \frac{3\varepsilon}{2\sqrt{2}} \partial_\nu \varphi \nabla_\tau \varphi = 0, \\ \mathbf{u} \cdot \nu = 0, \quad \mathbf{x} \in \partial\Omega,\ t > 0. \end{cases}$$

The inhomogeneous viscosity $\eta\,(\varphi)$ and mobility $M\,(\varphi)$ may produce specific boundary properties in the sharp interface limit, such as Navier slip boundary conditions [22].

Remark 21. In generalized Navier boundary conditions, the term $\sigma \frac{3\varepsilon}{2\sqrt{2}} \partial_\nu \varphi \partial_\tau \varphi$ is the so-called uncompensated Young stress. See [105] for expression in terms of contact angle and physical interpretation.

Remark 22. The case above considers the equilibrium contact angle [37, 109] to be $\pi/2$. For more general contact angle θ_c in [105], authors suggest boundary conditions

$$\begin{cases} \varphi_t + \mathbf{u}_\tau \cdot \nabla_\tau \varphi + \gamma \partial_\nu \varphi = 0, \quad \langle M\,(\varphi)\,\nabla\mu,\,\nu \rangle = 0, \\ \beta\,(\mathbf{u}_\tau) + \eta\,(\varphi)\,\partial_\nu\,(\mathbf{u}_\tau) - \lambda L\,(\varphi)\,\nabla_\tau \varphi = 0, \\ \mathbf{u} \cdot \nu = 0, \quad \mathbf{x} \in \partial\Omega,\ t > 0, \\ L\,(\varphi) = \partial_\nu \varphi + \partial \gamma_{fs}\,(\varphi)\,/\partial\varphi, \end{cases}$$

where $\gamma_{fs} = \frac{C_{fs}}{2} \cos\theta_c \sin\,(\pi\varphi/2)$ is an additional interfacial free energy density. The free energy considered in this case should be

$$\mathcal{F} = \lambda \left(\mathcal{W}\,(\varphi) + \int_{\partial\Omega} \gamma_{fs} dS_x \right).$$

5   Conclusion

The general energetic variational framework, with its energy dissipation laws, as well as the corresponding variational forms (weak forms), gives a self-consistent coupled system. It focuses on the coupling and competition of various parts of the mechanism, such as the energetics vs. kinematics, macroscopic (fields) vs. microscopic (configurations), and conservative forces vs. dissipative forces. It is a natural framework to study the multiscale and multiphysics problems. Moreover, such derivations are also very important in the analysis as well as the designing of numerical schemes in simulations.

There are two essential underlying hypothesis in the framework presented in this chapter. First, as described in Sect. 2.1, the procedure is only applicable to isothermal processes. For examples of non-isothermal complex fluid models, one may refer to [52, 87] and their references. Secondly, the dissipation $\mathcal{D}$ is limited to be quadratic in "rate," which is equivalent to the linear response theory in nonequilibrium thermodynamics [39, 74]. On one hand, this limitation is strong, and it does not allow considerations of some models, including Ostwald-de Waele type (power-law) fluids [40, 75, 108]. However, it is important to note that strong non-linearities can be introduced through coefficients not dependent on the "rate" (e.g., density-dependent viscosity). Also, some non-Newtonian structure of the fluid may be introduced through additional parameters (e.g., incompressible viscoelasticity system (22)).

This chapter only demonstrates the underlying variational structures for several complex fluid models. With the common energetic variational themes, each system possesses its own unique properties, hence difficulties and challenges: the viscoelastic fluids with its elastic mechanism (the transport of the deformation tensor), the mixtures with the interface evolutions (hence the dynamics of singularities), the diffusion with the complicated free energy and also the dissipative terms. All these are the motivation and challenges for researchers in both theoretical fields and in many interdisciplinary applications.

Energetic variational approaches have been successfully incorporated in many other important application not listed in this chapter, such as multicomponent flows with more than two phases [20–22], fracture mechanics [17, 129], and more. Contributions of the boundary effects, such as slip (Navier) boundary conditions [104, 105] and capacitors and surface chemistry [124], can also be incorporated in the variational framework. However, these boundary effects will bring in high gradients in the system and hence difficulties both in analysis and numerics.

For some of the models in this chapter analysis, results are presented in other chapters. Despite the constant efforts by many researchers, there are still many open problems in the area of complex fluids, as we can see in many other chapters. In particular, we want to point out the following areas for further research:

- For both micro-macro system (23) and Oldroyd-B equations that may be recovered from it, besides the difficulties of Navier-Stokes subsystem, the global existence of Leray-Hopf solutions and stability is mostly open;
- For phase field models in Sect. 4, further investigations may include: limit when interface thickness ε goes to zero, various dynamic boundary conditions and boundary effects, and various longtime stabilities.
- The understanding and reformulation of various weak forms of the system, with suitable test functions that are consistent with the energetic variational framework, such as the approaches of optimal transport for various diffusion equations.

6 Cross-References

▶ Classical Well-Posedness of Free Boundary Problems in Viscous Incompressible Fluid Mechanics
▶ Derivation of Equations for Continuum Mechanics and Thermodynamics of Fluids
▶ Equations for Polymeric Materials
▶ Equations for Viscoelastic Fluids
▶ Large Time Behavior of the Navier-Stokes Flow
▶ Modeling and Analysis of the Ericksen–Leslie Equations for Nematic Liquid Crystal Flows
▶ Models and Special Solutions of the Navier-Stokes Equations
▶ Multi-Fluid Models Including Compressible Fluids
▶ Singular Limits for Models of Compressible, Viscous, Heat Conducting, and/or Rotating Fluids
▶ Weak Solutions and Diffuse Interface Models for Incompressible Two-Phase Flows

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