Proceeding of the
36th Sapporo Symposium on Partial Differential Equations,
August 22 - 24, 2011, Faculty of Science, Hokkaido University.

Energetic Variational Approaches for Complex Fluids

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1 Complex fluids — fluids with microstructures

The most common origin and manifestation of anomalous phenomena in complex fluids are different "elastic" effects [29]. They can be the elasticity of deformable particles; elastic repulsion between charged liquid crystals, polarized colloids or multi-component 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 dumb-bell model for polymeric materials, the electric, magnetic field in electrorheological and magneto-hydrodynamic fluids, the volume fraction in mixture of different materials etc. The different rheological and hydrodynamic properties can be attributed to the special coupling between the kinematic transportation of the internal variable and the induced elastic stress. In our energetic formulation, this contributes to a competition between the kinetic energy and the elastic energy.

In complex fluids, it is the interaction between the (microscopic) elastic properties and the (macroscopic) fluid motions that gives not only the complicated rheological phenomena, but also formidable challenges in analysis and numerical simulations of the materials. In electro- and magneto-rheological fluids, material inhomogeneity and electro-magnetic effects can also lead to viscoelastic phenomena [29, 46, 6, 14]. In particular, how the deformation tensor F transports in the flow field and how elastic energy described by a functional of F, $W(F)$, competes with the kinetic energy in the flow play an important role in the study of complex fluids. In principle, the deformation tensor F carries all the transport/kinematic information of the microstructures, patterns and configurations in complex fluids.

As an example, for an isotropic viscoelastic fluid system, the following action functional summarizes the competition between the kinetic and elastic energy:

$$A(x) = \int_0^T \int_{\Omega_0} \frac{1}{2}\rho|x_t(X,t)|^2 - \lambda W(F)\, dX dt, \tag{1}$$

where $v = x_t(X,t)$ is the fluid velocity, $x(X,t)$ is the mapping between the Lagrange coordinate and the Eulerian coordinate system of the fluid, λ represents the ratio between the kinetic and elastic energies, Ω_0 is the original domain occupied by the material in the Lagrange coordinate. The fluid incompressibility implies $J = \det F = 1$. Using the Least Action Principle, we can derive the momentum transport equation [1, 2, 16, 29]:

$$\rho(v_t + v \cdot \nabla v) + \nabla p = \nabla \cdot \tau + f, \tag{2}$$

where p is the pressure, f is the external force density, and τ is the extra stress given by $\tau = \mu D(v) + \lambda(1/J)S(F)F^T$. Here $S(F) = [\partial W/\partial F]$ takes the Piola Kirchhoff form. The deformation tensor is transported through:

$$F_t + v \cdot \nabla F = \nabla v \cdot F. \tag{3}$$

These constitute a closed hydrodynamical system describing isotropic viscoelastic fluids. In the absence of the viscosity, the system provide an Eulerian description of incompressible elasticity [23, 38, 36]. In the case of "linear" elasticity, where $W(F) = \frac{H}{2}|F|^2 = \frac{H}{2}\mathrm{tr}(FF^T)$, the system describes the infinite Weissenberg number Oldroyd-B viscoelasticity [29, 42].

Note that the viscous stress can be derived by either postulating the dissipation functional and then using the Maximum Dissipation Principle [14, 20, 19, 17] or using the stochastic approach [43, 22]. The later is consistent with the fluctuation-dissipation theorem in thermodynamics [28]. With this, the system satisfies the energy estimate:

$$\frac{1}{2}\frac{d}{dt}\int_\Omega [\rho(\phi)|v|^2 + \lambda(1/J)W(F)]dx + \int_\Omega \mu(\phi)|D(v)|^2 dx = 0. \tag{4}$$

While the above viscoelastic models have been applied to various real materials, the study of other elastic complex fluids can be framed in an unified energetic variational approaches. Note that the above isotropic viscoelastic systems only reflect the transport part of the material. For other specific complex fluids, the elastic energy will take other more specific forms, in particular as those for MHD [12] and electro-kinetic fluids [44]. There the energy contributions will also take effects in the microscopic configuration and evolution equations.

2 EnVarA — Energetic Variational Approaches

The general energetic variational framework for classical mechanics had been developed by Rayleigh and Onsager in their seminal works published in 1873 [45] and 1936 [40].

In isothermal situations, a dissipative system satisfies the Second law of thermodynamics

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

where E^{total} is the total energy, including both the kinetic energy and the internal energy (in this case, we do not need to distinguish the Helmholtz free energy and the internal energy), and Δ is the dissipation functional which is equal to entropy production in this situation.

The Least Action Principle, which states that the equation of motion for a Hamiltonian system can be derived from the variation of the action functional with respect to the flow maps, is really the manifestations of the following general rule:

$$\delta E = force \cdot \delta x.$$

It gives a unique procedure to derive the conservative forces for the system.

The Maximum Dissipation Principle, variation of the dissipation functional with respect to the rate (such as velocity), gives the dissipative force for the system:

$$\delta\frac{1}{2}\Delta = force \cdot \delta u.$$

Basic mechanics. The good example to illustrate the procedure is the following Hookean spring model:

$$mx_{tt} + \gamma x_t + kx = 0.$$

The equation posses the following energy law:

$$\frac{d}{dt}(\frac{1}{2}mx_t^2 + \frac{1}{2}kx^2) = -\gamma x_t^2.$$

From the Hamiltonian, we can obtain the Lagrangian of the system $\int \frac{1}{2}mx_t^2 - \frac{1}{2}kx^2\,dt$. Employing the Least Action Principle, we arrive at the conservative part of the system.

The dissipative (damping) term is really by the Maximum Dissipation Principle, i.e. the variation of the dissipation with respect to the velocity.

The whole system is really the balance of all the forces. Notice the conservative part of the system really reflect the short time (near initial data) dynamics, the transient behavior of the whole dynamics. The dissipation part reflects the long time, near equilibrium, part of the dynamics. The choice of the dissipation functional, the quadratic form of the velocity, reflects the linear response theory for the near equilibrium dynamics.

Newtonian fluids. Next we look at the familiar model of the Navier-Stokes equation for incompressible Newtonian fluids:

$$u_t + u \cdot \nabla u + \nabla p = \mu \Delta u,$$

with incompressible constraint $\nabla \cdot u = 0$.

Again the system posses the energy law:

$$\frac{d}{dt}\int \frac{1}{2}|u|^2\,dx = -\int \mu |\nabla u|^2\,dx.$$

The Hamiltonian part of dynamics, from the Least Action Principle, is the Euler equation, which represents the short time (near initial data) dynamics. The dissipation part from the Maximum Dissipation Principle is the Stokes equation, for the long time dynamics near equilibrium.

Diffusion equations. Finally, we want to look at the following parabolic equations:

$$f_t = c\Delta f$$

. We rewrite the system into the following equivalent coupled system:

$$\begin{aligned} f_t + \nabla \cdot (uf) &= 0, \\ \nabla(cf) &= -fu. \end{aligned}$$

The first equation is just the common conservation of mass, which is just a change of variable from the Lagrangian particle coordinate to Eulerian coordinate. Set the left hand side $p = cf$, it immediate resembles to the Darcy's law, with compressible equation of states the same as that of ideal gas. Indeed, according to the first law of thermodynamics, the corresponding internal energy density will be $cf \ln f$. Moreover,

$$\frac{d}{dt}\int cf \ln f\,dx = -\int fu^2\,dx.$$

In fact, we can see that the force corresponding to the pressure $\nabla(cf)$ is obtained from the variation of the left hand side of the above equation with respect to the flow map x, while the dissipative force $-fu$ is from the variation of the right hand side with respect to the velocity u.

3 Electrorheological fluids and ionic solutions

How microstructures affect the bulk rheology of complex fluids is exemplified by electrorheological fluids. The hydrodynamical properties in a electrokinetic flow is determined by the coupling of the

transport of the concentration of the charges and the induced elastic force (the Lorentz force). The mathematical system can be illustrated in the following system [4, 5, 44, 11, 3, 47, 48]:

$$\rho(u_t + u \cdot \nabla u) + \nabla \pi = \nu \Delta u + (n - p)\nabla V, \quad \nabla \cdot u = 0, \tag{5}$$

$$n_t + u \cdot \nabla n = \nabla \cdot (D_n \nabla n - \mu_n n \nabla V), \tag{6}$$

$$p_t + u \cdot \nabla p = \nabla \cdot (D_p \nabla p + \mu_p p \nabla V), \tag{7}$$

$$\nabla \cdot (\epsilon \nabla V) = n - p. \tag{8}$$

Equations (5) represents the momentum equations where u is the fluid velocity, π is the pressure, ρ is the fluid density and ν the fluid viscocity. In equation (5), $(n-p)\nabla V$ is the macroscopic Lorentz (or Coulomb) force. Equations (6), (7) and (8) form the Nernst-Planck-Poisson system of a binary charge system, n and p are the densities of diffuse, negative and positive charges respectively. D_n, D_p are the respective diffusivity constants and μ_n, μ_p are the respective mobility constants. D_n, D_p and μ_n, μ_p are related by Einstein's relation and the valence of the charged particles.

The elastic energy combines both the electric energy and the entropy (contributes to the diffusion of the charge density). These different energy functions will generate various microstructures, as other elastic complex fluids. The induced Lorentz force is also due to the kinetic transport of the charged particles and electric energy balance.

The above system is very important in understanding the complicated behaviors relevant to electrophysiology.

In [49], we studied the stationary configurations of the stationary Ernest-Planck-Poisson equations and the limiting behavior as the (non-dimensional) Debye constant becomes small. We give the rigirous proof of the different Debye layer configuration between the electrial neutral and non-neutral cases [32]. These special boundary layer properties are crucial in the application [4, 5].

In [50] we reformulated the above hydrodynamical system of ER fluids, using different variational procedures. The method reveals the fundamental structures of the coupling and transport in these systems. We notice the work [41, 39] on the convection-diffusion equations. We obtained the well-posedness results of the system, based on our energetic variational approach. Moreover, combined with our diffusive interface methods, we developed systems/numerical algorithms to model the deformation of the vesicle membranes with preferable charge (ions) selections.

In [53], a hydrodynamical model for non-diluted ER fluids had been established and the numerical results had shown good agreements with the experimental data. We are studying the analytical properties on these system with nonlocal interactions or correlations and extend the theory to the ionic biological fluids and their interaction with proteins (ion channels) [24, 25].

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