Thermodynamically Consistent Models and Their Structure-Preserving Numerical Approximations

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References:

- Yuezheng Gong, Jia Zhao, and Qi Wang, An Energy Stable Algorithm for the Quasi-incompressible Hydrodynamic Model of Viscous Fluid Mixtures, Computer Physics Communications, 219 (2017), pp. 20-34.
- Xiaofeng Yang, Jia Zhao, and Qi Wang, Linear and Unconditionally Energy Stable Schemes for Molecular Beam Epitaxial Growth Model Based on Invariant Energy Quadratization Methods, Journal of Computational Physics, 333 (2017), pp. 104-127.
- Yuezheng Gong, Jia Zhao, and Qi Wang, Linear Second Order in Time Energy Stable Schemes for Hydrodynamic Models of Binary Mixtures Based on a Spatially Pseudospectral ApproximationAdvances in Computational Mathematics, accepted, 2018.
- Yuezheng Gong, Jia Zhao, Xiaogang Yang and Qi Wang, Second-order Linear Schemes for Hydrodynamic Phase Field Models of Binary Viscous Fluids with Variable Densities, Siam Journal on Scientific Computing, 40-1 (2018), pp. B138-B167.
- Yuezheng gong, Jia Zhao, and Qi Wang, Second Order Fully-Discrete Energy Stable Methods on Staggered Grids for Hydrodynamic Phase Field Models of Binary Viscous Fluids, Siam Journal on Scientific Computing, 40:2, B528-B553 (2018).
- Jia Zhao, Xiaofeng Yang, Yuezheng Gong, Xueping Zhao, Jun Li, Xiaogang Yang and Qi Wang, A General Strategy for Numerical Approximations of Thermodynamically Consistent Nonequilibrium Models–Part I: Thermodynamical Systems, International Journal of Numerical Analysis and Modeling, accepted, 2018.
- Jia Zhao, Yuezheng Gong and Qi Wang. Arbitrarily High Order Unconditionally Energy Stable Schemes for Gradient Flow Models. Submitted to Journal of Computational Physics, 2018.

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Thermodynamically consistent models and their approximations

Thermodynamically consistent models

A reasonable dynamical model describing non-equilibrium phenomena must be derived following thermodynamical principles and conservation laws (unfortunately, there are some ad hoc models which do not follow this rule.)

- Thermodynamical principles: first, second law of thermodynamics.
- First law: energy conservation.
- Second law: positive entropy production.
- Equivalent formulations: Onsager principle, GENERIC formalism, Poisson bracket formulation, EVAR formulation, Onsager-Matchlup action potential formulation etc.
- Additional conservation laws: mass, linear momentum, angular momentum conservation.
- If electromagnetic effects are included, Maxwell equations need to be coupled.

We call these laws constraints. Models derived subject to the above constraints are called thermodynamically consistent models.

Structure-preserving numerical approximations

The numerical algorithms that respect some or all the above constraints are called the structure-preserving numerical approximations.

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A simple example: heat equation

Let e be the internal energy, T the absolute temperature and V a material domain. The energy conservation in the material volume states that

$$\frac{d}{dt} \int_{V} e d\mathbf{x} = -\int_{\partial V} \mathbf{n} \cdot \mathbf{q} dS, \qquad (1.1)$$

where **n** is the unit external normal of the boundary ∂V and **q** is the heat flux. Its differential form is

$$\frac{de}{dt} = -\nabla \cdot \mathbf{q}. \tag{1.2}$$

Fourier law (constitutive relation):

$$\mathbf{q} = -k\nabla T,\tag{1.3}$$

where k is a constant measuring the heat flux. We assume

$$e = e(T_0) + C(T - T_0),$$
 (1.4)

near a constant temperature T_0 , where $C = \frac{\partial e}{\partial T}|_{T_0}$ is the specific heat. Denote $\theta = T - T_0$. Then,

$$\theta_t = D\nabla^2 \theta \tag{1.5}$$

is the model for heat conduction, where $D = \frac{k}{C}$ is the heat conductivity.

Consider the heat equation in a domain Ω subject to the boundary condition $\theta|_{\partial\Omega} = 0$ or $\frac{\partial\theta}{\partial \mathbf{n}}|_{\Omega} = 0$. Define the energy as $E = \int_{\Omega} \frac{\theta^2}{2} d\mathbf{x}$. Then,

$$\frac{dE}{dt} = -\int_{\Omega} D \|\nabla\theta\|^2 d\mathbf{x}$$
(1.6)

where the right hand side is called the energy dissipation rate. It implies

$$E(t) \le E(0). \tag{1.7}$$

It implies

$$\|\theta(t)\|_{2} \le \|\theta(0)\|_{2} \tag{1.8}$$

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where $\|\theta\|_2 = (\int_{\Omega} \theta^2 d\mathbf{x})^{1/2}$ is the L_2 norm.

Energy dissipation \Rightarrow well-posedness of the equation.

Energy stable schemes-schemes preserves the energy dissipation property

We discretize the equation in time using Crank-Nicolson scheme

$$\frac{\theta^{n+1} - \theta^n}{\Delta t} = D\nabla^2 \theta^{n+1/2},\tag{1.9}$$

where $\theta^{n+1/2} = \frac{\theta^{n+1}+\theta^n}{2}$.

$$E^{n+1} - E^n = \Delta t \int_{\Omega} \theta^{n+1/2} D\nabla^2 \theta^{n+1/2} d\mathbf{x} = -\Delta t \int_{\Omega} D \|\nabla \theta^{n+1/2}\|^2 d\mathbf{x}.$$
 (1.10)

So,

$$E^{n+1} \le E^n. \tag{1.11}$$

Schemes satisfy this property is called energy stable scheme. It implies

$$\|\theta^n\|_2 \le \|\theta^0\|_2. \tag{1.12}$$

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So, the numerical scheme is even stable. But, for nonlinear PDEs in general, this may not be established.

Generalized Onsager Principle–A constructive tool for deriving models for nonequilibrium systems?

- Generalized Onsager Principle (GOP) (Onsager, 1931, 1933, Joanny et al, 2007, Yang & Wang 2015). Key ingredients: the free energy or entropy and the mobility matrix. The former provides the energy landscape while the latter selects the path to equilibrium states, which defines the so-called dynamics.
- Application of GOP to thermodynamic systems \Rightarrow gradient flows.
- Application of GOP to generalized hydrodynamics ⇒ constitutive equations are gradient flows.
- Application of GOP to electrolytic hydrodynamics ⇒ constitutive equation, including the Omh's law.
- Many more applications....
- There are other formalisms: GENERIC (Ottinger & Grmela, 1997, 2000), Poisson Bracket (Beris & Edwards, 1994), Energetic Variational Methods (Ericksen, 1961, Leslie, 1979, Chun Liu, et al. 2006-present), Second law of thermodynamics, Onsager maximum entropy approach for dissipative systems (Onsager, 1933, Doi et al, 2014).

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Generalized Onsager Principle

Let \mathbf{x} be the state variable vector, containing internal variables and others.

- Free energy is a functional of the state variables,
- $\mathbf{M} = \mathbf{M}_{sym} + \mathbf{M}_{anti}$ is a differential or integral operator depending on the thermodynamic variables,
- The kinetic equation,

$$\dot{\mathbf{x}} = \mathbf{M} \cdot \mathbf{X},\tag{2.13}$$

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where \mathbf{X} is the conjugate force of \mathbf{x} . Then,

$$\frac{dF}{dt} = -const \times \int \mathbf{X} \cdot \dot{\mathbf{x}} = -const \times \int \mathbf{X} \cdot \mathbf{M} \cdot \mathbf{X}, \qquad (2.14)$$

where *F* is the free energy of the system.

- reciprocal relation: $\mathbf{M}_{anti} = 0$ for purely dissipative systems,
- dissipative property: $\mathbf{M}_{sym} > 0$ so that $\dot{F} < 0$.

It is an essential tool to derive the constitutive relation for matter systems.

Application to Dissipative Thermodynamic Systems

Free energy:

$$F = \int f(\{\phi_i\}, \{\nabla\phi_i\}, \{\nabla^2\phi_i\}, \cdots) d\mathbf{x}, \qquad (2.15)$$

where $\phi_i, i = 1, \dots, n-1$ are the phase variables. The energy dissipation is given by

$$\frac{dF}{dt} = \int (\mu_1, \cdots, \mu_m) \cdot (\dot{\phi_1}, \cdots, \dot{\phi_m})^T d\mathbf{x}.$$
(2.16)

where $\mu_i = \frac{\delta f}{\delta \phi_i}$, $i = 1, \cdots, m$ are chemical potentials. Generalized onsager principle implies

$$(\dot{\phi}_1,\cdots,\dot{\phi}_m)^T = -\mathbf{M}\cdot(\mu_1,\cdots,\mu_m)^T, \qquad (2.17)$$

where $\mathbf{M} = \mathbf{M}_{sym}$ is the mobility matrix.

• M is algebraic \Rightarrow Allen-Cahn systems.

•
$$\mathbf{M} = -\nabla \mathbf{L} \nabla (\mu_1, \cdots, \mu_m)^T \Rightarrow \text{Cahn-Hilliard systems.}$$

• $\frac{dF}{dt} = -\int (\mu_1, \cdots, \mu_m) \cdot \mathbf{M}_{sym} \cdot (\mu_1, \cdots, \mu_m) dx.$

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Application to Non-dissipative Systems (Nonlinear Schrodinger equation)

Let u be a complex function. Consider the energy

$$F = \int [\nabla u \cdot \nabla \bar{u} + V(|u|)] dx, \qquad (2.18)$$

where V(|u|) is a potential function.

$$\frac{dF}{dt} = \int \left[u_t \left(-\nabla^2 \bar{u} + \frac{\partial V}{\partial |u|^2} \bar{u} \right) + \bar{u}_t \left(-\nabla^2 u + \frac{\partial V}{\partial |u|^2} u \right) \right] dx.$$
(2.19)

Set

$$u_t = M(-\nabla^2 u + \frac{\partial V}{\partial |u|^2}u).$$
(2.20)

 $\frac{dF}{dt} = 0 \Rightarrow$

$$M = M_{anti} = \pm i. \tag{2.21}$$

Nonlinear Schrodinger equation:

$$iu_t = \nabla^2 u - \frac{\partial V}{\partial |u|^2} u. \tag{2.22}$$

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Application to Generalized Hydrodynamics

Objective: develop a general framework to derive hydrodynamic theories for complex fluids/soft matter systems via variation+generalized Onsager principle.

Let ρ , **v**, σ and **F**_e be the mass density, velocity, total stress, and total body force of the system.

• Mass conservation:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0.$$

• Momentum conservation

$$\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) = \nabla \cdot \boldsymbol{\sigma} + \mathbf{F}_{\mathbf{e}}.$$

Constitutive equation accounting for the microstructure of the system for σ and F_e. This includes: σ and F_e, functionals of internal variables, and transport equations for the internal variables.

Remark: The singular limits of the momentum equation like the Stokes equation can be handled analogously using the Onsager maximum entropy principle.

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Example: a general hydrodynamic theory for binary complex fluids

Mass conservation:

Consider a mixture of complex fluids, whose micro-structures are described by the first 3 moments $(c, \mathbf{p}, \mathbf{Q})$ of a microstructural distribution function and solvent with the total mass density ρ and mass averaged velocity \mathbf{v} . The mass conservation is given by

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{v}) = 0. \tag{2.23}$$

c: number density of the microscopic constituent in the complex fluid. Then,

$$\partial_t c + \nabla \cdot (c \mathbf{v} + \mathbf{j}) = 0, \qquad (2.24)$$

where **j** is an extra diffusive flux.

Momentum conservation:

$$\frac{\partial(\rho \mathbf{v})}{\partial t} = \nabla \cdot \boldsymbol{\sigma} + \mathbf{F}_e. \tag{2.25}$$

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where σ is the total stress (momentum flux) and \mathbf{F}_e is the elastic force.

Constitutive equations:

Derive evolution equations for $c, \mathbf{p}, \mathbf{Q}$ and constitutive equation for flux **j**, stress σ and \mathbf{F}_e .

Derivation of constitutive equations (cf: Joanny etal. NJP, 2007)

Free energy

$$F = F[c, \nabla c, \mathbf{p}, \nabla \mathbf{p}, \mathbf{Q}, \nabla \mathbf{Q}] = \int_{V} f(c, \nabla c, \mathbf{p}, \nabla \mathbf{p}, \mathbf{Q}, \nabla \mathbf{Q}) dV.$$
(2.26)

Total "mechanical free energy": $E^{total} = \int_{V} [\frac{\rho}{2} ||\mathbf{v}||^2 + f] dV$. The energy dissipation rate at a constant temperature *T*:

$$\frac{dE^{total}}{dt} = \int_{V} \{ \frac{1}{2} \frac{\partial(\rho \|\mathbf{v}\|^{2})}{\partial t} + \frac{\partial f}{\partial t} \} dV = \int_{V} [-\nabla \cdot (\frac{\rho \mathbf{v}}{2} \|\mathbf{v}\|^{2}) + \mathbf{v} \cdot (\nabla \cdot \sigma + \mathbf{F}_{e}) + \mu \frac{\partial c}{\partial t} - \mathbf{h} \cdot \frac{\partial \mathbf{p}}{\partial t} - \mathbf{G} : \frac{\partial \mathbf{Q}}{\partial t} \} dV =$$

$$(2.27)$$

$$\int_{\partial V} \left[-\frac{\rho \mathbf{n} \cdot \mathbf{v}}{2} \|\mathbf{v}\|^2 + \mathbf{v} \cdot \boldsymbol{\sigma} \cdot \mathbf{n} - \mathbf{n} \cdot \mathbf{j}\mu\right] ds + \int_{V} \left[-\mathbf{D} \cdot \boldsymbol{\sigma}^s + \nabla \mu \cdot \mathbf{j} - \mathbf{h} \cdot \dot{\mathbf{P}} - \mathbf{G} : \overline{\mathbf{Q}}\right] dV,$$

where $\mu = \frac{\delta F}{\delta c}$, $\mathbf{h} = -\frac{\delta F}{\delta \mathbf{p}}$, $\mathbf{G} = -\frac{\delta F}{\delta \mathbf{Q}}$, σ^a : antisymmetric stress, σ^e Ericksen stress, and σ^s symmetric stress,

$$\sigma_{\alpha\beta}^{s} = \sigma_{\alpha\beta} - \sigma_{\alpha\beta}^{e} - \sigma_{\alpha\beta}^{a}, \quad D_{\alpha\beta} = \frac{1}{2}(\partial_{\alpha}v_{\beta} + \partial_{\beta}v_{\alpha}), \quad \Omega_{\alpha\beta} = \frac{1}{2}(\partial_{\alpha}v_{\beta} - \partial_{\beta}v_{\alpha}), \quad (2.28)$$

$$\dot{c} = \partial_t c + \nabla \cdot (\mathbf{v}c), \quad \dot{P}_{\alpha} = \partial_t p_{\alpha} + v_{\beta} \partial_{\beta} p_{\alpha} + \Omega_{\alpha\beta} p_{\beta}, \quad \mathbf{Q} = \frac{\partial \mathbf{Q}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{Q} + [\Omega \cdot \mathbf{Q} - \mathbf{Q} \cdot \Omega].$$

$$\sigma_{\alpha\beta}^{a} = \frac{1}{2} (p_{\alpha}h_{\beta} - p_{\beta}h_{\alpha}) + (Q_{\alpha\gamma}G_{\gamma\beta} - G_{\alpha\gamma}Q_{\gamma\beta}), \qquad (2.29)$$

$$\partial_{\beta}\sigma^{e}_{\alpha\beta} = -(c\partial_{\alpha}\mu + h_{\gamma}\partial_{\alpha}p_{\gamma} + G_{\beta\gamma}\partial_{\alpha}Q_{\beta\gamma}).$$
(2.30)

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$$E^{iotal} = -\int_{V} (\sigma^{s}, \mathbf{Q}, \dot{\mathbf{P}}, \mathbf{j}) \cdot (\mathbf{D}, \mathbf{G}, \mathbf{h}, -\nabla \mu)^{T} dV, \qquad (2.31)$$

where

$$\begin{array}{cccc} & & & & & & \\ \Box \\ (\sigma^{s}_{\alpha\beta}, Q_{\alpha\beta}, \dot{P}_{\alpha}, j_{\alpha}) & \longleftrightarrow & (D_{\alpha\beta}, G_{\alpha\beta}, h_{\alpha}, -\partial_{\alpha}\mu). \end{array}$$

$$(2.32)$$

Generalized Onsager principle:

$$G-Fluxes = [\mathbf{M}_{sym} + \mathbf{M}_{anti}] \cdot G-Force$$

The total mechanical energy dissipation rate:

$$\frac{d}{dt} \int_{V} E^{total} d\mathbf{x} = -\int_{V} T\dot{S} d\mathbf{x} = -\int Force \cdot \mathbf{M}_{sym} \cdot Force d\mathbf{x}.$$
(2.33)

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Example 1: Binary viscous fluid mixture model

We ignore \mathbf{p} and \mathbf{Q} and only consider c as the internal variable.

$$\begin{pmatrix} \sigma^{\nu} \\ \mathbf{j} \end{pmatrix} = \mathbf{M} \cdot \begin{pmatrix} \mathbf{D} \\ -\nabla\mu \end{pmatrix}, \sigma^{a} = 0, \nabla \cdot \sigma^{e} = -c\nabla\mu, \sigma^{s} = -p\mathbf{I} + \sigma^{\nu}$$
(2.34)

where

$$\mathbf{M} = \begin{pmatrix} 2\eta \delta_{\alpha k} \delta_{\beta l} & \\ 0 & \lambda \delta_{\alpha k} \end{pmatrix}, \tag{2.35}$$

 η and $\bar{\eta}$ are viscosity coefficients and λ is the mobility. The governing system of equations is given by

$$\frac{\partial c}{\partial t} + \nabla (c\mathbf{v}) + \nabla \cdot \lambda \cdot \nabla \mu = 0,
\nabla \cdot \mathbf{v} = 0,
\rho(\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v}) = -\nabla p - c\nabla \mu + \nabla \cdot \sigma^{s},$$
(2.36)

where ρ is a prescribed function of c and c can be normalized to be a volume fraction or a mass fraction. This is known as the Navier-Stokes-Cahn-Hilliard system.

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Example 2: Quasilinear model for viscoelastic fluids

We consider only \mathbf{Q} as the internal variable.

$$\sigma^{s} = \sigma^{v} - p\mathbf{I}, \begin{pmatrix} \sigma^{v} \\ \Box \\ \mathbf{Q} \end{pmatrix} = \mathbf{M} \cdot \begin{pmatrix} \mathbf{D} \\ \mathbf{G} \end{pmatrix}$$
(2.37)

where

$$\mathbf{M}_{sym} = \begin{pmatrix} 2\eta \delta_{\alpha k} \delta_{\beta l} & 0\\ 0 & \frac{1}{\lambda} \delta_{\alpha k} \delta_{\beta l} \end{pmatrix},$$
(2.38)

 γ_2 is the relaxation time.

$$\mathbf{M}_{anti} = \begin{pmatrix} 0 & -A_1 \\ A_1 & 0 \end{pmatrix}, \tag{2.39}$$

$$A_1 = a[Q_{\alpha k}\delta_{\beta l} + \delta_{\alpha k}Q_{\beta l}].$$

The governing system of equations is given by

$$\begin{aligned}
\overset{\sqcup}{\mathbf{Q}} &- a[\mathbf{D} \cdot \mathbf{Q} + \mathbf{Q} \cdot \mathbf{D}] - \frac{1}{\lambda} \mathbf{G} = 0, \\
\nabla \cdot (\mathbf{v}) &= 0, \\
\rho(\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v}) &= -\nabla p + \nabla \cdot (\sigma^s - \sigma^e - \sigma^a),
\end{aligned}$$
(2.40)

where ρ is a constant. If a proper free energy density is defined, Oldroyd B model is recovered.

Example 3: Binary quasi-incompressible viscous fluid mixture model

We denote **u** the mass average velocity. The governing system of equations in the quasi-incompressible fluid mixture model is given below.

$$\rho(\partial_t \mathbf{v} + \mathbf{v} \cdot \nabla \mathbf{v}) = -\nabla p + \nabla \cdot \tau - \phi \nabla \mu,$$

$$\nabla \cdot \mathbf{v} = a \nabla \cdot (\lambda \nabla (\mu + ap)),$$

$$\partial_t \phi + \nabla \cdot (\phi \mathbf{v}) = \nabla \cdot (\lambda \nabla (\mu + ap)),$$

(2.41)

where

•
$$a = 1 - \frac{\rho_1}{\rho_2}$$
, $\rho_{1,2}$ are constant mass density of fluid A and B,

•
$$\rho = \rho_1 \phi + \rho_2 (1 - \phi)$$
 is the total mass density,

- $\tau = 2\eta \mathbf{D} + \nu \mathrm{tr}(\mathbf{D})\mathbf{I}$,
- the shear viscosity $\eta = \eta_1 \phi + \eta_2 (1 \phi)$,
- the volumetric viscosity $\nu = \nu_1 \phi + \nu_2 (1 \phi)$.

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Numerical approximations-EQ

Goals of numerical approximations to PDE systems:

Derive discrete schemes to approximate the continuous system so that

- a solution exists and converges to that of the continuous system;
- the discrete solution keeps "as close to the continuous system as possible". This includes: preserving the mass, volume, and sign of certain variables required by their physical meaning (positivity preserving), conserving certain physical quantities like certain invariants and energy dissipation laws etc.
- Namely, the discrete numerical approximation should mimic the continuous system.

Numerical methods and estimates:

- Energy stable schemes: the numerical approximations for the system that respect the energy dissipation at the corresponding rate.
- Positivity preserving scheme: preserves positivity of c and non-negative definiteness of $\mathbf{Q} + \frac{c\mathbf{I}}{3}$. (partially open)
- Error estimates and convergence (Open).
- The discrete system should be solved efficiently. Therefore, linear schemes are preferred.

Novel Numerical Techniques: EQ

Introduce new intermediate or auxiliary variables to transform the free energy into a polynomial form. A quadratic energy form will yield a linear scheme, others, nonlinear scheme. GOP provides a paradigm for us to do it.

Basic idea of EQ for a thermodynamic model

Consider a thermodynamic model

$$\phi_t = \mathbf{M} \cdot \boldsymbol{\mu}, \tag{3.42}$$

where M: mobility and $\mu = \frac{\delta F}{\delta \phi}$: chemical potential. Introducing an intermediate variable q s.t.

$$F = \int_{V} \frac{1}{2}q^{2}d\mathbf{x} + const.$$
(3.43)

Then, $\mu = qq'$ and

$$q_t = q'\phi_t. \tag{3.44}$$

From the equations of ϕ and q, we obtain the energy dissipation rate:

$$\int_{t_n}^{t_{n+1}} F_t dt = \int_{t_n}^{t_{n+1}} \int_V \frac{q^2_t}{2} d\mathbf{x} dt = \int_{t_n}^{t_{n+1}} \int_V \mu M \mu d\mathbf{x}.$$
 (3.45)

We discretize the equations as follows

$$\phi^{n+1} - \phi^n = \overline{Mq'}^{n+1/2} q^{n+1/2} (t_{n+1} - t_n), \quad q^{n+1} - q^n = \overline{q'}^{n+1/2} \int_{t_n}^{t_{n+1}} \phi_t d\mathbf{x}.$$
(3.46)

We have a second order energy stable scheme. We multiply the first by $q^{n+1/2}\overline{q'}^{n+1/2}$ and the second by $q^{n+1/2}$, add them up to get the discrete energy dissipation rate:

$$F^{n+1} - F^n = \Delta t \int_V \overline{q'}^{n+1/2} q^{n+1/2} \cdot \overline{\mathbf{M}}^{n+1/2} \cdot \overline{q'}^{n+1/2} q^{n+1/2} d\mathbf{x}$$
(3.47)

Reformulation of thermodynamic models using the EQ method In general, we consider the total free energy given by

$$F = \frac{1}{2}(\Phi, \mathcal{L}\Phi) + (f(\Phi), 1), \qquad (3.48)$$

where \mathcal{L} is a linear, self-adjoint, positive definite operator and f is the rest of the free energy density, which is bounded from below for physically accessible state of Φ . Then

$$F = \frac{1}{2}(\Phi, \mathcal{L}\Phi) + \frac{1}{2} ||q||^2 - A, \quad q = \sqrt{2\left(f + \frac{A}{|\Omega|}\right)},$$
(3.49)

where A is a constant large enough to make q well-defined. Then

$$\left\{\begin{array}{c}\frac{\partial}{\partial t}\Phi = M\left(\mathcal{L}\Phi + q\frac{\partial q}{\partial \Phi}\right), \quad \frac{\partial}{\partial t}q = \frac{\partial q}{\partial \Phi} : \frac{\partial \Phi}{\partial t}.\end{array}\right.$$
(3.50)

Denoting $\Psi = (\Phi, q)^T$,

$$\frac{\partial}{\partial t}\Psi = \mathcal{N}\mathcal{B}\Psi,\tag{3.51}$$

where $\mathcal{N} = \mathcal{A}^* M \mathcal{A}$, \mathcal{A}^* is an adjoint operator of \mathcal{A} , and

$$\mathcal{A} = (\mathbf{I}_n \quad \frac{\partial q}{\partial \Phi})_{n,n+1}, \quad \mathcal{B} = diag(\mathcal{L}, 1)_{n+1,n+1}.$$

For the case $q = q(\Phi)$, we have $\mathcal{A}^* = \mathcal{A}^T$. In addition, \mathcal{B} is a linear, self-adjoint, positive definite operator. The energy dissipation law

$$\frac{dF}{dt} = \left(\frac{\delta F}{\delta \Psi}, \frac{\partial \Psi}{\partial t}\right) = \left(\mathcal{B}\Psi, \mathcal{N}\mathcal{B}\Psi\right) \le 0. \quad \text{for all } t \in \mathbb{R}, \quad t \in \mathbb$$

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First and second order unconditionally energy stable, linear schemes

Scheme (First Order, Linear Backward Difference Scheme)

Given the initial condition Ψ^0 and having computed Ψ^n , we compute Ψ^{n+1} as follows:

$$\frac{\Psi^{n+1} - \Psi^n}{\Delta t} = \mathcal{N}(\Psi^n) \mathcal{B} \Psi^{n+1}.$$
(3.53)

Scheme (Second Order, Linear Backward Difference Scheme)

Given the initial condition Ψ^0 , we first compute Ψ^1 by Scheme 3.1. Having computed Ψ^{n-1} and Ψ^n , we compute Ψ^{n+1} as follows:

$$\frac{3\Psi^{n+1} - 4\Psi^n + \Psi^{n-1}}{2\Delta t} = \mathcal{N}(\overline{\Psi}^{n+1})\mathcal{B}\Psi^{n+1}, \quad \overline{(\bullet)}^{n+1} = 2(\bullet)^n - (\bullet)^{n-1}.$$
 (3.54)

Scheme (Second Order, Linear Crank-Nicolson scheme)

Given the initial condition Ψ^0 , we first compute Ψ^1 by Scheme 3.1. Having computed Ψ^{n-1} and Ψ^n , we compute Ψ^{n+1} as follows:

$$\frac{\Psi^{n+1} - \Psi^n}{\Delta t} = \mathcal{N}(\overline{\Psi}^{n+\frac{1}{2}})\mathcal{B}\Psi^{n+\frac{1}{2}}, (\bullet)^{n+\frac{1}{2}} = \frac{1}{2}(\bullet)^{n+1} + \frac{1}{2}(\bullet)^n, \overline{(\bullet)}^{n+\frac{1}{2}} = \frac{3}{2}(\bullet)^n - \frac{1}{2}(\bullet)^{n-1}.$$
(3.55)

Prediction-correction type unconditionally energy stable methods

Scheme (Second Order, Linear, Fixed-point type Prediction-Correction BDF2 Scheme)

Given the initial condition Ψ^0 , we first compute Ψ^1 by Scheme 3.1. Having computed Ψ^{n-1} and Ψ^n . Set $\Psi_0^{n+1} = 2\Psi^n - \Psi^{n-1}$. Given a chosen positive integer N and error tolerance ϵ_0 : for *i* in 0 to N - 1, while $\|\Psi_{i+1}^{n+1} - \Psi_i^{n+1}\| > \epsilon_0$, we solve for Ψ_{i+1}^{n+1} via

$$\frac{3\Psi_{i+1}^{n+1} - 4\Psi^n + \Psi^{n-1}}{2\Delta t} = \mathcal{N}(\Psi_i^{n+1})\mathcal{B}\Psi_{i+1}^{n+1}.$$
(3.56)

If the loop breaks at Ψ_k^{n+1} , $k \leq N$, we assign Ψ^{n+1} by $\Psi^{n+1} = \Psi_k^{n+1}$.

Scheme (Second Order, Linear, Fixed-point type Prediction-Correction CN Scheme)

Given the initial condition Ψ^0 and having computed Ψ^n , we set $\Psi_0^{n+1} = \Psi^n$. Given a chosen positive integer N and error tolerance ϵ_0 : for i in 0 to N - 1, while $\|\Psi_{i+1}^{n+1} - \Psi_i^{n+1}\| > \epsilon_0$, we solve for Ψ_{i+1}^{n+1} via

$$\frac{\Psi_{i+1}^{n+1} - \Psi^n}{\Delta t} = \mathcal{N}\Big(\frac{\Psi_i^{n+1} + \Psi^n}{2}\Big)\mathcal{B}\frac{\Psi_{i+1}^{n+1} + \Psi^n}{2}.$$
(3.57)

If the loop breaks at Ψ_k^{n+1} , $k \leq N$, we assign Ψ^{n+1} by $\Psi^{n+1} = \Psi_k^{n+1}$.

High order linear schemes

We define the backward difference operator for the *k*th order derivative as follows:

$$\Lambda_k \Psi^{n+1} = \sum_{i=0}^k \lambda_i^k \Psi^{n+1-i},$$
(3.58)

where $\Lambda_0 \Psi^{n+1} := \Psi^{n+1}$. Then, we propose the BDF-*k* scheme (with *k* the order of the scheme)

Scheme (BDF-k) Given values for $\Psi^{n+1-k}, \Psi^{n+2-k}, \dots, \Psi^n$, we obtain Ψ^{n+1} via $\frac{1}{\Delta t} \Lambda_k \Psi^{n+1} = \mathcal{N}(\overline{\Psi}^{n+1}) \mathcal{B} \Psi^{n+1}$, (3.59) where $\overline{(\bullet)}^{n+1}$ is either an explicit extrapolation with values of previous time steps or we can use

where $(\bullet)^{n+1}$ is either an explicit extrapolation with values of previous time steps or we can use some predictors.

Unfortunately, we are not able to prove the scheme to be unconditionally energy stable, although in practice it is shown to deliver an energy decay numerical result for gradient flows.

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Arbitrarily high order, unconditionally energy stable schemes We denote system (3.51) as

$$\frac{\partial}{\partial t}\Psi = g(\Psi), \text{ with } \Psi(t=0) = \Psi_0,$$
(3.60)

where $g(\Psi) = \mathcal{N}(\Psi)\mathcal{B}\Psi$.

Scheme (s-stage RK Method)

Let b_i , a_{ij} $(i, j = 1, \dots, s)$ be real numbers and let $c_i = \sum_{j=1}^{s} a_{ij}$. Given Ψ^n , Ψ^{n+1} is calculated by

$$k_{i} = g(\Psi^{n} + \Delta t \sum_{j=1}^{s} a_{ij}k_{j}), \quad i = 1, \cdots, s,$$

$$\Psi^{n+1} = \Psi^{n} + \Delta t \sum_{i=1}^{s} b_{i}k_{i}.$$
(3.61)

The coefficients are usually displayed by a Butcher table

$$\frac{\mathbf{c} \mid \mathbf{A}}{\mathbf{b}^{T}} = \frac{\begin{array}{ccc} c_{1} & a_{11} & \cdots & a_{1s} \\ \vdots & \vdots & & \vdots \\ \hline c_{s} & a_{s1} & \cdots & a_{ss} \\ \hline b_{1} & \cdots & b_{s} \end{array}$$

where $\mathbf{A} \in \mathbb{R}^{s,s}$, $\mathbf{b} \in \mathbb{R}^{s}$, and $\mathbf{c} = \mathbf{A}\mathbf{l}$, with $\mathbf{l} = (1, 1, \cdots, 1)^{T} \in \mathbb{R}^{s}$.

Applying an *s*-stage collocation method to (3.60), we obtain the following scheme.

Scheme (s-stage Collocation Method)

Let c_1, \dots, c_s be distinct real numbers (usually $0 \le c_i \le 1$). Given Ψ^n , the collocation polynomial u(t) is a polynomial of degree s satisfying

$$u(t_n) = \Psi^n,$$

$$\dot{u}(t_n + c_i \Delta t) = g(u(t_n + c_i \Delta t)), \quad i = 1, \cdots, s,$$
(3.62)

and the numerical solution is defined by $\Psi^{n+1} = u(t_n + \Delta t)$.

Lemma

The above two schemes are equivalent with coefficients of the RK schemes given by

$$a_{ij} = \int_0^{c_i} l_j(\tau) d\tau, \quad b_i = \int_0^1 l_i(\tau) d\tau, \tag{3.63}$$

where $l_i(\tau)$ is the Lagrange interpolation polynomial $l_i(\tau) = \prod_{l \neq i} \frac{\tau - c_l}{c_i - c_l}$.

Theorem

All Gaussian collocation methods are unconditionally energy stable, i.e., they satisfy the following energy law

$$F^{n+1} - F^n = \Delta t \sum_{i=1}^s b_i \Big(\mathcal{B}u(t_n + c_i \Delta t), \mathcal{N}\big(u(t_n + c_i \Delta t)\big) \mathcal{B}u(t_n + c_i \Delta t) \Big) \le 0, \qquad (3.64)$$

where $F^n = \frac{1}{2} ||\Psi^n||_{\mathcal{B}}^2 - A$, c_i $(i = 1, \dots, s)$ are the Gaussian quadrature nodes, $b_i \ge 0$ $(i = 1, \dots, s)$ are the Gauss-Legendre quadrature weights given in (3.63), u(t) be the collocation polynomial of the Gaussian collocation methods.

For general RK methods, we have the following theorem.

Theorem

If the coefficients of a RK method satisfy

$$b_i a_{ij} + b_j a_{ji} = b_i b_j, \quad b_i \ge 0, \quad \forall \ i, j = 1, \cdots, s,$$
 (3.65)

then it is unconditionally energy stable, i.e., it satisfies the following energy law

$$F^{n+1} - F^n = \Delta t \sum_{i=1}^s b_i \Big(\mathcal{B}\Psi_i, \mathcal{N}(\Psi_i) \mathcal{B}\Psi_i \Big) \le 0,$$
(3.66)

Solvability and a numerical example: crystal growth

Solvability: The linear schemes are solvable uniquely provided the PDEs are solvable.

Example: the free energy is given by

$$F = \int_{\Omega} d\mathbf{x} \Big[\frac{1}{4} \phi^4 + \frac{a - \eta}{2} \phi^2 - a |\nabla \phi|^2 + \frac{1}{2} (\Delta \phi)^2 \Big],$$
(3.67)

where ϕ is the phase variable, *a* and η are two model parameters. The transport equation for ϕ is given by

$$\begin{cases} \partial_t \phi = \nabla \cdot (M_\phi \nabla \mu), \\ \mu = \phi^3 + (a - \eta)\phi + 2a\Delta\phi + \Delta^2\phi. \end{cases}$$
(3.68)

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4th order RK results on crystal growth model



Figure: The phase field crystal growth dynamics at times t = 10, 20, 30, 50, 100, 1000.

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Stability vs accuracy in a CH model simulation of a rounding droplet



Figure: The energy in time period [0, 2] calculated using various schemes. (a) The regular CN Scheme 3.3 with different time step sizes. (b) The fixed point CN Scheme 3.5 with different time step sizes. (c) The 4th order Gauss scheme with different time step sizes. (d) The 6th order Gauss scheme with different time step sizes.

Incompressible Hydrodynamic Binary Fluid Model

The hydrodynamic model consists of the following coupled partial differential equations:

$$\begin{cases} \rho \Big(\partial_t \mathbf{v} + \mathbf{v} \cdot \nabla \mathbf{v} \Big) = -\nabla p + \nabla \cdot \tau - \phi \nabla \mu, \\ \nabla \cdot \mathbf{v} = 0, \\ \partial_t \phi + \nabla \cdot (\phi \mathbf{v}) = \nabla \cdot (M \nabla \mu), \end{cases}$$
(3.69)

where **u** is the mass-average velocity, ϕ is the phase variable, p is the hydrostatic pressure, $\mu = \frac{\delta F}{\delta \phi}$ is the chemical potential, $\tau = 2\eta \mathbf{D}$ is the viscous stress tensor with viscosity η , $\mathbf{D} = \frac{1}{2}(\nabla \mathbf{v} + \nabla \mathbf{v}^T)$ is the rate of strain tensor, ρ is the total mass density, M is the mobility.

Boundary condition:

- $\mathbf{u}|_{\partial\Omega} = \mathbf{0}, \mathbf{n} \cdot \nabla \phi|_{\partial\Omega} = 0, \mathbf{n} \cdot \nabla \mu|_{\partial\Omega} = 0.$
- Or, the periodic boundary condition.

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Energy Dissipation

The free energy of the mixture system is given by

$$F[\phi] = \int_{\Omega} \left(\frac{\gamma_1}{2} |\nabla \phi|^2 + f(\phi) \right) d\mathbf{x}, \qquad (3.70)$$

which gives $\mu = f'(\phi) - \gamma_1 \Delta \phi$.

• Double well repulsive potential:

$$f(\phi) = \gamma_2 \phi^2 (1 - \phi)^2.$$
 (3.71)

• Flory-Huggins free energy density:

$$f(\phi) = \gamma_2 \left(\frac{\phi}{N_1} \ln \phi + \frac{(1-\phi)}{N_2} \ln(1-\phi) + \chi \phi(1-\phi)\right).$$
(3.72)

Energy dissipation law:

$$\frac{d}{dt}E = -\int_{\Omega} [2\eta \mathbf{D} : \mathbf{D} + M |\nabla \mu|^2] d\mathbf{x}.$$
(3.73)

where $E = \int_{\Omega} \left[\frac{\rho}{2} |\mathbf{v}|^2 + \frac{\gamma_1}{2} |\nabla \phi|^2 + f(\phi)\right] d\mathbf{x}.$

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Reformulation to an equivalent hydrodynamic system

In order to develop energy dissipative algorithm, system (3.69) can be written equivalently to the following form:

$$\begin{cases} \rho \Big(\partial_t \mathbf{v} + \frac{1}{2} \big(\mathbf{v} \cdot \nabla \mathbf{v} + \nabla \cdot (\mathbf{v} \mathbf{v}) \big) \Big) = -\nabla p + \eta \Delta \mathbf{v} - \phi \nabla \mu, \\ \nabla \cdot \mathbf{v} = 0, \\ \partial_t \phi + \nabla \cdot (\phi \mathbf{v}) = M \Delta \mu, \end{cases}$$
(3.74)

where $\mathbf{v} \cdot \nabla \mathbf{v} = \frac{1}{2} (\mathbf{v} \cdot \nabla \mathbf{v} + \nabla \cdot (\mathbf{v}\mathbf{v}))$ was used due to $\nabla \cdot \mathbf{u} = 0$.

• Y. Gong, X. Liu and Q. Wang, Fully Discretized Energy Stable Schemes for Hydrodynamic Equations Governing Two-phase Viscous Fluid Flows, J. Sci. Comput., DOI 10.1007/s10915-016-0224-7, 2016.

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Spatial discretization-finite differences

Discrete difference operators:

$$\begin{split} \delta_{x}^{+}f_{j,k} &= \frac{f_{j+1,k} - f_{j,k}}{h_{x}}, \delta_{x}^{-}f_{j,k} = \frac{f_{j,k} - f_{j-1,k}}{h_{x}}, \delta_{\overline{x}}f_{j,k} = \frac{\delta_{x}^{+} + \delta_{x}^{-}}{2}f_{j,k}, \\ \delta_{y}^{+}f_{j,k} &= \frac{f_{j,k+1} - f_{j,k}}{h_{y}}, \delta_{\overline{y}}^{-}f_{j,k} = \frac{f_{j,k} - f_{j,k-1}}{h_{y}}, \delta_{\overline{y}}f_{j,k} = \frac{\delta_{y}^{+} + \delta_{y}^{-}}{2}f_{j,k}, \\ \nabla_{h}^{+} &= \begin{pmatrix} \delta_{x}^{+} \\ \delta_{y}^{+} \end{pmatrix}, \nabla_{h}^{-} = \begin{pmatrix} \delta_{x}^{-} \\ \delta_{y}^{-} \end{pmatrix}, \overline{\nabla}_{h} = \frac{\nabla_{h}^{+} + \nabla_{h}^{-}}{2}, \Delta_{h} = \delta_{x}^{+}\delta_{x}^{-} + \delta_{y}^{+}\delta_{y}^{-}. \end{split}$$

Discrete inner product and norm:

$$(\mathbf{F}, \mathbf{G})_{h} = \sum_{m,n} \sum_{j=0}^{N_{x}-1} \sum_{k=0}^{N_{y}-1} (\mathbf{F}_{m,n})_{j,k} (\mathbf{G}_{m,n})_{j,k} h_{x} h_{y}, \quad \|\mathbf{F}\|_{h} = (\mathbf{F}, \mathbf{F})_{h}^{1/2}.$$

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Spatially discretized scheme

$$\begin{cases} \rho\left(\frac{d}{dt}\mathbf{v}_{j,k} + \frac{1}{2}\left(\mathbf{v}_{j,k}\cdot\overline{\nabla}_{h}\mathbf{v}_{j,k} + \overline{\nabla}_{h}\cdot\left(\mathbf{v}_{j,k}\mathbf{v}_{j,k}\right)\right)\right) = -\overline{\nabla}_{h}p_{j,k} + \eta\Delta_{h}\mathbf{v}_{j,k} - \phi_{j,k}\overline{\nabla}_{h}\mu_{j,k},\\ \overline{\nabla}_{h}\cdot\mathbf{v}_{j,k} = 0,\\ \frac{d}{dt}\phi_{j,k} + \overline{\nabla}_{h}\cdot\left(\phi_{j,k}\mathbf{v}_{j,k}\right) = M\Delta_{h}\mu_{j,k}, \end{cases}$$
(3.75)

where $\mu_{j,k} = f'(\phi_{j,k}) - \gamma_1 \Delta_h \phi_{j,k}$ and $j = 0, 1, \dots, N_x - 1, k = 0, 1, \dots, N_y - 1$.

Theorem

The scheme (3.75) preserves the following energy identity

$$\frac{dE_h}{dt} + \eta \|\nabla_h^+ \mathbf{v}\|_h^2 + M \|\nabla_h^+ \mu\|_h^2 = 0, \qquad (3.76)$$

where E_h is the discrete energy functional defined as

$$E_{h} = \frac{\rho}{2} \|\mathbf{v}\|_{h}^{2} + \frac{\gamma_{1}}{2} \|\nabla_{h}^{+}\phi\|_{h}^{2} + (f(\phi), 1)_{h}.$$

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Fully implicit nonlinear scheme

$$\begin{cases} \delta_{t}^{+} \mathbf{v}_{j,k}^{n} + \frac{1}{2} \big(\mathbf{v}_{j,k}^{n+1/2} \cdot \overline{\nabla}_{h} \mathbf{v}_{j,k}^{n+1/2} + \overline{\nabla}_{h} \cdot \big(\mathbf{v}_{j,k}^{n+1/2} \mathbf{v}_{j,k}^{n+1/2} \big) \big) \\ = -\overline{\nabla}_{h} p_{j,k}^{n+1/2} + \eta \Delta_{h} \mathbf{v}_{j,k}^{n+1/2} - \phi_{j,k}^{n+1/2} \overline{\nabla}_{h} \mu_{j,k}^{n,n+1}, \\ \overline{\nabla}_{h} \cdot \mathbf{v}_{j,k}^{n} = 0, \\ \delta_{t}^{+} \phi_{j,k}^{n} + \overline{\nabla}_{h} \cdot \big(\phi_{j,k}^{n+1/2} \mathbf{v}_{j,k}^{n+1/2} \big) = M \Delta_{h} \mu_{j,k}^{n,n+1}, \end{cases}$$
(3.77)

where

$$\begin{split} \mu_{j,k}^{n,n+1} &= \frac{\delta f}{\delta(\phi_{j,k}^{n+1},\phi_{j,k}^n)} - \gamma_1 \Delta_h \phi_{j,k}^{n+1/2},\\ \frac{\delta f}{\delta(a,b)} &= \begin{cases} \frac{f(a)-f(b)}{a-b}, & \text{if } a \neq b,\\ f'(a), & \text{if } a = b. \end{cases} \end{split}$$

Theorem

The fully discretized scheme (3.77) preserves the discrete energy identity

$$\delta_t^+ E_h^n + \eta \|\nabla_h^+ \mathbf{v}^{n+1/2}\|_h^2 + M \|\nabla_h^+ \mu^{n,n+1}\|_h^2 = 0,$$
(3.78)

where

$$E_h^n = \frac{1}{2} \|\mathbf{v}^n\|_h^2 + \frac{\gamma_1}{2} \|\nabla_h^+ \phi^n\|_h^2 + (f(\phi^n), 1)_h.$$

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Energy quadratization reformulation

In order to reformulation an energy quadratic model for the system (3.74), we introduce a new variable

$$q = \sqrt{f(\phi)},\tag{3.79}$$

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where we assume f > 0, and rewrite the system (3.74) as follows:

$$\begin{cases} \rho \Big(\partial_t \mathbf{v} + \frac{1}{2} \big(\mathbf{v} \cdot \nabla \mathbf{v} + \nabla \cdot (\mathbf{v} \mathbf{v}) \big) \Big) = -\nabla p + \eta \Delta \mathbf{v} - \phi \nabla \mu, \\ \nabla \cdot \mathbf{v} = 0, \\ \partial_t \phi + \nabla \cdot (\phi \mathbf{v}) = M \Delta \mu, \\ \partial_t q = g(\phi) \partial_t \phi, \end{cases}$$
(3.80)

where
$$\mu = 2qg(\phi) - \gamma_1 \Delta \phi$$
 and $g(\phi) = \frac{f'(\phi)}{2\sqrt{f(\phi)}}$.

Linear-implicit Scheme

$$\begin{cases} \delta_{t}^{+} \mathbf{v}_{j,k}^{n} + \frac{1}{2} (\overline{\mathbf{v}}_{j,k}^{n+1/2} \cdot \overline{\nabla}_{h} \mathbf{v}_{j,k}^{n+1/2} + \overline{\nabla}_{h} \cdot (\mathbf{v}_{j,k}^{n+1/2} \overline{\mathbf{v}}_{j,k}^{n+1/2})) \\ = -\overline{\nabla}_{h} p_{j,k}^{n+1/2} + \eta \Delta_{h} \mathbf{v}_{j,k}^{n+1/2} - \overline{\phi}_{j,k}^{n+1/2} \overline{\nabla}_{h} \mu_{j,k}^{n,n+1}, \\ \overline{\nabla}_{h} \cdot \mathbf{v}_{j,k}^{n} = 0, \\ \delta_{t}^{+} \phi_{j,k}^{n} + \overline{\nabla}_{h} \cdot (\overline{\phi}_{j,k}^{n+1/2} \mathbf{v}_{j,k}^{n+1/2}) = M \Delta_{h} \mu_{j,k}^{n,n+1}, \\ \delta_{t}^{+} q_{j,k}^{n} = \overline{g(\phi_{j,k})}^{n+1/2} \delta_{t}^{+} \phi_{j,k}^{n}, \end{cases}$$
(3.81)
where $\mu_{j,k}^{n,n+1} = 2q_{j,k}^{n+1/2} \overline{g(\phi_{j,k})}^{n+1/2} - \gamma_{1} \Delta_{h} \phi_{j,k}^{n+1/2} \text{ and} \\ \delta_{t}^{+} u^{n} = \frac{u^{n+1} - u^{n}}{\Delta t}, \ u^{n+1/2} = \frac{u^{n+1} + u^{n}}{2}, \ \overline{u}^{n+1/2} = \frac{1}{2}(3u^{n} - u^{n-1}). \end{cases}$

Theorem

The fully discrete scheme (3.81) preserves the discrete energy identity

$$\delta_t^+ E_h^n + \eta \|\nabla_h^+ \mathbf{v}^{n+1/2}\|_h^2 + M \|\nabla_h^+ \mu^{n,n+1}\|_h^2 = 0, \qquad (3.82)$$

where

$$E_h^n = \frac{1}{2} \|\mathbf{v}^n\|_h^2 + \frac{\gamma_1}{2} \|\nabla_h^+ \phi^n\|_h^2 + \|q^n\|_h^2.$$

Quasi-incompressible viscous fluid mixture model

In order to reformulate an equivalent model with a quadratic energy functional, we introduce two new variables $\mathbf{u} = \sqrt{\rho} \mathbf{v}$, $q = \sqrt{f(\phi)}$ where we assume f > 0, and rewrite the quasi-incompressible system as follows:

$$\partial_t \mathbf{u} + \frac{1}{2} \left(\mathbf{u} \cdot \nabla(\frac{\mathbf{u}}{\sqrt{\rho}}) + \frac{1}{\sqrt{\rho}} \nabla \cdot (\mathbf{u} \mathbf{u}) \right) = \frac{1}{\sqrt{\rho}} (-\nabla p + \nabla \cdot \tau - \phi \nabla \mu), \qquad (3.83a)$$

$$\nabla \cdot \left(\frac{\mathbf{u}}{\sqrt{\rho}}\right) = a\nabla \cdot \left(\lambda \nabla(\mu + ap)\right),\tag{3.83b}$$

$$\partial_t \phi + \nabla \cdot \left(\frac{1}{\sqrt{\rho}} \phi \mathbf{u}\right) = \nabla \cdot \left(\lambda \nabla (\mu + ap)\right),\tag{3.83c}$$

$$\partial_t q = g(\phi)\partial_t \phi, \tag{3.83d}$$

where the chemical potential μ becomes $\mu = 2qg(\phi) - \gamma_1 \Delta \phi$, $g(\phi) = \frac{f'(\phi)}{2\sqrt{f(\phi)}}$.

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A nonlinear energy stable scheme

$$\delta_{t}^{+} \mathbf{u}_{j,k}^{n} + \frac{1}{2} \left(\mathbf{u}_{j,k}^{n+\frac{1}{2}} \cdot \overline{\nabla}_{h} \left(\left(\frac{1}{\sqrt{\rho}} \right)_{j,k}^{n+\frac{1}{2}} \mathbf{u}_{j,k}^{n+\frac{1}{2}} \right) + \left(\frac{1}{\sqrt{\rho}} \right)_{j,k}^{n+\frac{1}{2}} \overline{\nabla}_{h} \cdot \left(\mathbf{u}_{j,k}^{n+\frac{1}{2}} \mathbf{u}_{j,k}^{n+\frac{1}{2}} \right) \right) \\ = \left(\frac{1}{\sqrt{\rho}} \right)_{j,k}^{n+\frac{1}{2}} \left(-\overline{\nabla}_{h} p_{j,k}^{n+\frac{1}{2}} + \overline{\nabla}_{h} \cdot \tau_{j,k}^{n,n+1} - \phi_{j,k}^{n+\frac{1}{2}} \overline{\nabla}_{h} \mu_{j,k}^{n,n+1} \right),$$
(3.84a)

$$\overline{\nabla}_{h} \cdot \left(\left(\frac{1}{\sqrt{\rho}} \right)_{j,k}^{n+\frac{1}{2}} \mathbf{u}_{j,k}^{n+\frac{1}{2}} \right) = a \overline{\nabla}_{h} \cdot \left(\lambda_{j,k}^{n+\frac{1}{2}} \overline{\nabla}_{h} \left(\mu_{j,k}^{n,n+1} + a p_{j,k}^{n+\frac{1}{2}} \right) \right), \tag{3.84b}$$

$$\delta_{\iota}^{+}\phi_{j,k}^{n} + \overline{\nabla}_{h} \cdot \left(\left(\frac{1}{\sqrt{\rho}}\right)_{j,k}^{n+\frac{1}{2}}\phi_{j,k}^{n+\frac{1}{2}} \mathbf{u}_{j,k}^{n+\frac{1}{2}} \right) = \overline{\nabla}_{h} \cdot \left(\lambda_{j,k}^{n+\frac{1}{2}}\overline{\nabla}_{h}(\mu_{j,k}^{n,n+1} + ap_{j,k}^{n+\frac{1}{2}})\right),$$
(3.84c)

where

$$\begin{aligned} \mathbf{D}_{j,k}^{n,n+1} &= \frac{1}{2} \left(\overline{\nabla}_{h} \left(\left(\frac{1}{\sqrt{\rho}} \right)_{j,k}^{n+\frac{1}{2}} \mathbf{u}_{j,k}^{n+\frac{1}{2}} \right) + \overline{\nabla}_{h} \left(\left(\frac{1}{\sqrt{\rho}} \right)_{j,k}^{n+\frac{1}{2}} \mathbf{u}_{j,k}^{n+\frac{1}{2}} \right)^{T} \right), \\ \tau_{j,k}^{n,n+1} &= 2\eta_{j,k}^{n+\frac{1}{2}} \mathbf{D}_{j,k}^{n,n+1} + \nu_{j,k}^{n+\frac{1}{2}} \operatorname{tr}(\mathbf{D}_{j,k}^{n,n+1}) \mathbf{I}, \\ \mu_{j,k}^{n,n+1} &= \frac{\delta f}{\delta(\phi_{j,k}^{n+1}, \phi_{j,k}^{n})} - \gamma_{1} \Delta_{h} \phi_{j,k}^{n+\frac{1}{2}}, \quad \frac{\delta f}{\delta(a,b)} = \begin{cases} \frac{f(a) - f(b)}{a - b}, & \text{if } a \neq b, \\ f'(a), & \text{if } a = b, \end{cases} \end{aligned}$$

and $j = 0, 1, \dots, N_x - 1, k = 0, 1, \dots, N_y - 1, n = 0, 1, \dots, N_t - 1.$

Theorem

Under the assumption of the periodic boundary condition, scheme (3.84) preserves the discrete energy dissipation law

$$\delta_t^+ E^n + (\lambda^{n+\frac{1}{2}}, |\overline{\nabla}_h(\mu^{n,n+1} + ap^{n+\frac{1}{2}})|^2)_h + 2(\eta^{n+\frac{1}{2}}, |\mathbf{D}^{n,n+1}|^2)_h + (\nu^{n+\frac{1}{2}}, |tr(\mathbf{D}^{n,n+1})|^2)_h = 0,$$
(3.85)

where E^n is the discrete energy defined as

$$E^{n} = \frac{1}{2} \|\mathbf{u}^{n}\|_{h}^{2} + \frac{\gamma_{1}}{2} \|\nabla_{h}^{+}\phi^{n}\|_{h}^{2} + (f(\phi^{n}), 1)_{h}.$$

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A linear energy stable scheme

$$\delta_{t}^{+} \mathbf{u}_{j,k}^{n} + \frac{1}{2} \left(\overline{\mathbf{u}}_{j,k}^{n+\frac{1}{2}} \cdot \overline{\nabla}_{h} \left(\overline{\left(\frac{1}{\sqrt{\rho}}\right)}_{j,k}^{n+\frac{1}{2}} \mathbf{u}_{j,k}^{n+\frac{1}{2}} \right) + \overline{\left(\frac{1}{\sqrt{\rho}}\right)}_{j,k}^{n+\frac{1}{2}} \overline{\nabla}_{h} \cdot \left(\mathbf{u}_{j,k}^{n+\frac{1}{2}} \overline{\mathbf{u}}_{j,k}^{n+\frac{1}{2}} \right) \right)$$
$$= \overline{\left(\frac{1}{\sqrt{\rho}}\right)}_{i,k}^{n+\frac{1}{2}} \left(-\overline{\nabla}_{h} p_{j,k}^{n+\frac{1}{2}} + \overline{\nabla}_{h} \cdot \tau_{j,k}^{n,n+1} - \overline{\phi}_{j,k}^{n+\frac{1}{2}} \overline{\nabla}_{h} \mu_{j,k}^{n,n+1} \right), \qquad (3.86a)$$

$$\overline{\nabla}_{h} \cdot \left(\overline{\left(\frac{1}{\sqrt{\rho}}\right)}_{j,k}^{n+\frac{1}{2}} \mathbf{u}_{j,k}^{n+\frac{1}{2}} \right) = a \overline{\nabla}_{h} \cdot \left(\overline{\lambda}_{j,k}^{n+\frac{1}{2}} \overline{\nabla}_{h} (\mu_{j,k}^{n,n+1} + a p_{j,k}^{n+\frac{1}{2}}) \right),$$
(3.86b)

$$\delta_{t}^{+}\phi_{j,k}^{n} + \overline{\nabla}_{h} \cdot \left(\overline{\left(\frac{1}{\sqrt{\rho}}\right)}_{j,k}^{n+\frac{1}{2}} \overline{\phi}_{j,k}^{n+\frac{1}{2}} \mathbf{u}_{j,k}^{n+\frac{1}{2}}\right) = \overline{\nabla}_{h} \cdot \left(\overline{\lambda}_{j,k}^{n+\frac{1}{2}} \overline{\nabla}_{h} (\mu_{j,k}^{n,n+1} + ap_{j,k}^{n+\frac{1}{2}})\right), \quad (3.86c)$$

$$\delta_t^+ q_{j,k}^n = \overline{g(\phi)}_{j,k}^{n+\frac{1}{2}} \delta_t^+ \phi_{j,k}^n, \tag{3.86d}$$

where

$$\mathbf{D}_{j,k}^{n,n+1} = \frac{1}{2} \left(\overline{\nabla}_h \left(\overline{\left(\frac{1}{\sqrt{\rho}}\right)}_{j,k}^{n+\frac{1}{2}} \mathbf{u}_{j,k}^{n+\frac{1}{2}} \right) + \overline{\nabla}_h \left(\overline{\left(\frac{1}{\sqrt{\rho}}\right)}_{j,k}^{n+\frac{1}{2}} \mathbf{u}_{j,k}^{n+\frac{1}{2}} \right)^T \right),$$

$$\tau_{j,k}^{n,n+1} = 2\overline{\eta}_{j,k}^{n+\frac{1}{2}} \mathbf{D}_{j,k}^{n,n+1} + \overline{\nu}_{j,k}^{n+\frac{1}{2}} \operatorname{tr}(\mathbf{D}_{j,k}^{n,n+1}) \mathbf{I},$$

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Theorem

Scheme (3.86) preserves the discrete energy dissipation law

$$\delta_t^+ E^n + (\overline{\lambda}^{n+\frac{1}{2}}, |\overline{\nabla}_h(\mu^{n,n+1} + ap^{n+\frac{1}{2}})|^2)_h + 2(\overline{\eta}^{n+\frac{1}{2}}, |\mathbf{D}^{n,n+1}|^2)_h + (\overline{\nu}^{n+\frac{1}{2}}, |tr(\mathbf{D}^{n,n+1})|^2)_h = 0,$$
(3.87)

where the discrete energy is defined as

$$E^{n} = \frac{1}{2} \|\mathbf{u}^{n}\|_{h}^{2} + \frac{\gamma_{1}}{2} \|\nabla_{h}^{+} \phi^{n}\|_{h}^{2} + \|q^{n}\|_{h}^{2}.$$
(3.88)

Remark: The results apply to the models subject to physical boundary conditions on a staggered grid.

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Solvability of the linear systems obtained using linear schemes

Theorem

The linear schemes developed using EQ subject to periodic boundary conditions or on staggered-grid are uniquely solvable.

A lighter droplet in a heavier fluid:



Figure: A lighter viscous fluid drop rising in a heavier viscous fluid matrix. This figure illustrates the interface evolution at different time. The contour of $\phi = 0.5$ (the interface of the fluid drop) at time t = 0, 25, 75, 125 are shown in red. The blue color represents the background fluid matrix.

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Conclusions

- A paradigm for model development and numerical algorithm design is discussed in the name of GOP and EQ, respectively.
- The generalized Onsager principle is a useful tool for the development of models for nonequilibrium phenomena. Many previous models can be shown as special cases.
- Linear energy stable numerical schemes are developed for the nonequilibrium systems derived using the GOP and the new energy quadratization technique. This technique bypasses the stabilization and convex splitting technique to yield linear schemes.
- The numerical approximations have been done for a host of complex fluid models.
- The modeling and numerical approach are systematic and applicable to a large class of problems in science and engineering.

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