

Maximum dissipation principle in numerical simulation of complex fluids

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- Complex Fluids
- Energetic Variational Approaches on Simple Fluid
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- Numerical Results in Finite Element Methods
- Remarks

- Macroscopic fluids with microscopic configuration/structure
- Competition between the kinetic energy and the internal “elastic” energy
- Intrinsically multiscale-multiphysics model, or multicomponent

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- **Viscoelastic Fluids** (Polymeric Materials, Liquid Crystal,...)
- **Electrorheological (ER) Fluids** (Ion Dynamics(Electrolyte Solutions) in Biology, Semiconductor,...)
- **Magnetohydrodynamical (MHD) Fluids**
- **Multi-phase Flows** (Fluid-Fluid Mixture)

- The analysis of complex fluids is intrinsically difficult.
- Numerical computations are highly demanded to understand the complex fluids.
- The starting point of energetic variational approaches: Energy dissipation law for the whole coupled system,

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

where E^{total} is the total energy, Δ is the dissipation of the system.

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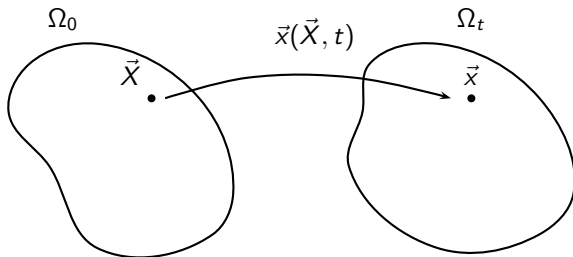


Figure: The flow map from the reference domain, Ω_0 to the current domain, Ω_t .

- **Basic Mechanics**

- Flow Map (Trajectory) : $\vec{x}_t(\vec{X}, t) = \vec{u}(\vec{x}(\vec{X}, t), t)$, $\vec{x}(\vec{X}, 0) = \vec{X}$.
- The deformation tensor (strain) of the flow map :

$$F(\vec{x}(\vec{X}, t), t) = \frac{\partial \vec{x}(\vec{X}, t)}{\partial \vec{X}} \text{ satisfying}$$

$$F_t + \vec{u} \cdot \nabla F = \nabla \vec{u} F. \quad (1)$$

- Least Action Principle (Hamilton's Principle; Principle of Virtual Work) : the reversible part of the system, conservative force (f_c)

$$\delta\mathcal{A} = f_c \cdot \delta\vec{x}$$

where \mathcal{A} is the action functional defined from the energy.

- Maximum Dissipation Principle¹ (Onsager's Principle) : the irreversible part of the system, the dissipative force (f_d)

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

- Force Balance Law through the energy law

¹L. ONSAGER, *Reciprocal Relations in Irreversible Processes I*, Phys. Rev. 37(1931), pp.405–426, *Reciprocal Relations in Irreversible Processes II*, Phys. Rev. 38(1931), pp. 2265–2279, L. ONSAGER, AND S. MACHLUP, *Fluctuations and Irreversible Processes*, Phys. Rev. 91(1953), pp. 1505–1512.

- **Simple Fluid** : the fluid described by the incompressible Navier-Stokes equations

$$\begin{aligned}\rho(\vec{u}_t + \vec{u} \cdot \nabla \vec{u}) + \nabla p &= \mu \Delta \vec{u}, & (\text{momentum conservation}) \\ \nabla \cdot \vec{u} &= 0, & (\text{incompressibility}) \\ \rho_t + \nabla \cdot (\rho \vec{u}) &= 0. & (\text{mass conservation})\end{aligned} \quad (2)$$

where ρ is mass, \vec{u} is velocity field, p is pressure, and μ is the viscosity.

- The energy equation for incompressible Navier-Stokes equation:

$$\frac{d}{dt} \int \frac{1}{2} \rho |\vec{u}|^2 d\vec{x} = - \int \mu |\nabla \vec{u}|^2 d\vec{x}. \quad (3)$$

- The total energy, the dissipation :

$$E^{total} = \int \frac{1}{2} \rho |\bar{\mathbf{u}}|^2 d\vec{x}, \quad \Delta = \int \mu |\nabla \bar{\mathbf{u}}|^2 d\vec{x}, \quad (4)$$

Energetic Variational Approaches : Simple Fluid

- Define Action Functional, \mathcal{A} , for Least Action Principle (LAP)

$$\mathcal{A} = \int_0^T \int_{\Omega_t} \frac{1}{2} \rho |\vec{u}|^2 d\vec{x} dt. \quad (5)$$

- Pull back the current domain, Ω_t , to the reference one, Ω_0 , through the flow map, $\vec{x}(\vec{X}, t)$

$$\mathcal{A}(\vec{x}) = \int_0^T \int_{\Omega_0} \frac{1}{2} \frac{\rho_0(\vec{X})}{\det F} |\vec{x}_t|^2 \det F d\vec{X} dt \quad (6)$$

where $\rho_0(\vec{X}) = \rho(\vec{X}, t)|_{t=0}$ is the initial mass. Then $\frac{\delta \mathcal{A}(\vec{x})}{\delta \vec{x}} = 0$ gives the Hamiltonian (energy conserved) part under the incompressibility condition, $\nabla \cdot \vec{u} = 0$, i.e., $\det(F) = 1$.

- The resulting equation is the Euler equation : the total energy conservation

$$\begin{aligned} \rho(\vec{u}_t + \vec{u} \cdot \nabla \vec{u}) &= -\nabla p \\ \nabla \cdot \vec{u} &= 0. \end{aligned} \quad (7)$$

- Applying Maximum Dissipation Principle (MDP) for the dissipation in the form of the quadratic of the “rate” functions,

$$\frac{1}{2} \frac{\delta \Delta}{\delta \vec{u}} \Big|_{\varepsilon=0} = \int (\nabla \vec{u} + \varepsilon \nabla \vec{v}) \cdot \nabla \vec{v} \, d\vec{x} \Big|_{\varepsilon=0} = 0,$$

then we obtain the Stokes equation,

$$\begin{aligned} \mu \Delta \vec{u} &= \nabla \tilde{p}, \\ \nabla \cdot \vec{u} &= 0. \end{aligned} \tag{8}$$

- Combine (7) and (8) then we have the incompressible Navier-Stokes equation (2)

Energetic Variational Approaches : Framework

- 1 Define an appropriate energy equation for describing the physical phenomenon.
- 2 Applying energetic variational approaches, LAP, MDP.
- 3 Combine the conservative part from LAP and the dissipative part from MDP through the force balance to satisfy the energy law.(The system of PDE is uniquely determined.)
- 4 Numerical Computations, developing numerical methods, existence, uniqueness of solutions

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- Immiscible Two-phase Flow²:

- Let ϕ be a phase function $\phi(\vec{x}, t) = \pm 1$ in the incompressible fluids
- Let $\Gamma_t = \{x : \phi(\vec{x}, t) = 0\}$ be the interface of mixture
- In the Eulerian description, the immiscibility of fluids implies the pure transport of ϕ .

$$\phi_t + \vec{u} \cdot \nabla \phi = 0. \quad (9)$$

²C. LIU, AND J. SHEN, *A Phase Field Model for the Mixture of Two Incompressible Fluids and Its Approximation by a Fourier-Spectral Method*, Physica D, 179(2003), pp.211–228.

- Immiscible Two-phase Flow:

- Ginzburg-Landau mixing energy, represents a competition between two fluids with their (hydro-) philic and (hydro-) phobic properties:

$$W(\phi, \nabla\phi) = \frac{1}{2}|\nabla\phi|^2 + \frac{1}{4\eta^2}(\phi^2 - 1)^2.$$

The equilibrium profile of interface is tanh-like function as $\eta \rightarrow 0$.

- The total energy is defined by the combination of the kinetic energy and the internal energy as follows:

$$E^{total} = \int_{\Omega_t} \left\{ \frac{1}{2}|\vec{u}|^2 + \lambda W(\phi, \nabla\phi) \right\} d\vec{x}. \quad (10)$$

where λ is the contribution coefficient of the mixing energy to the total energy.

- Immiscible Two-phase Flow:

- The action functional \mathcal{A} from the total energy (10):

$$\mathcal{A} = \int_0^T \int_{\Omega_t} \left\{ \frac{1}{2} |\vec{x}_t|^2 - \lambda W(\phi, \nabla \phi) \right\} d\vec{x} dt. \quad (11)$$

- The action functional \mathcal{A} in terms of the flow map:

$$\mathcal{A}(\vec{x}) = \int_0^T \int_{\Omega_0} \left\{ \frac{1}{2} |\vec{x}_t|^2 - \lambda \left(\frac{1}{2} |F^{-1} \nabla_{\vec{x}} \phi|^2 + f(\phi_0) \right) \det F \right\} d\vec{X} dt. \quad (12)$$

where $f(\phi_0) = \frac{1}{4\eta^2} |\phi_0^2 - 1|^2$.

- Immiscible Two-phase Flow without Dissipation:

- the LAP leads us to the following Hamiltonian system:

$$\vec{u}_t + \vec{u} \cdot \nabla \vec{u} + \nabla \tilde{p} = -\lambda \nabla \cdot (\nabla \phi \otimes \nabla \phi) \quad (13)$$

$$\nabla \cdot \vec{u} = 0 \quad (14)$$

$$\phi_t + \vec{u} \cdot \nabla \phi = 0. \quad (15)$$

- The above system (18) – (20) converges to the “sharp interface model” and its energy equation is

$$\frac{d}{dt} \int \left\{ \frac{1}{2} |\vec{u}|^2 + \lambda \left(\frac{1}{2} |\nabla \phi|^2 + \frac{1}{4\eta^2} (\phi^2 - 1)^2 \right) \right\} d\vec{x} = 0. \quad (16)$$

: the total energy conservation, a Hamiltonian system, a conservative force with no dissipation of system.

- Immiscible Two-phase Flow:

- Consider the following dissipation with the viscosity of fluids and the dissipation within the diffusive interface:

$$\Delta = \int \left(\mu |\nabla \vec{u}|^2 + \lambda \gamma \left| \Delta \phi - \frac{1}{\eta^2} (\phi^2 - 1) \phi \right|^2 \right) d\vec{x}. \quad (17)$$

where γ is the relation time. Since the dissipation of the diffusive interface is not a rate square, the maximum dissipation principle gives only the viscosity term, $\mu \Delta \vec{u}$.

- Immiscible Two-phase Flow:

- The system with dissipation:

$$\vec{u}_t + \vec{u} \cdot \nabla \vec{u} + \nabla \tilde{p} = \mu \Delta \vec{u} - \lambda \nabla \cdot (\nabla \phi \otimes \nabla \phi) \quad (18)$$

$$\nabla \cdot \vec{u} = 0 \quad (19)$$

$$\phi_t + \vec{u} \cdot \nabla \phi = \gamma \left(\Delta \phi - \frac{1}{\eta^2} (\phi^2 - 1) \phi \right). \quad (20)$$

- The dissipative energy law is

$$\begin{aligned} \frac{d}{dt} \int \left\{ \frac{1}{2} |\vec{u}|^2 + \lambda \left(\frac{1}{2} |\nabla \phi|^2 + \frac{1}{4\eta^2} (\phi^2 - 1)^2 \right) \right\} d\vec{x} \\ = - \int \left(\mu |\nabla \vec{u}|^2 + \lambda \gamma \left| \Delta \phi - \frac{1}{\eta^2} (\phi^2 - 1) \phi \right|^2 \right) d\vec{x}. \end{aligned} \quad (21)$$

- In numerical computation applying finite element methods one might need at least H^2 finite element space to satisfying the energy law.

- Immiscible Two-phase Flow with Dissipation:

Reducing the computational cost in numerical experiment through the Maximum dissipation principle.

- Manipulate the dissipation (17) in terms of a rate

$$\Delta = \int \left(\mu |\nabla \vec{u}|^2 + \frac{\lambda}{\gamma} |\phi_t + \vec{u} \cdot \nabla \phi|^2 \right) d\vec{x}. \quad (22)$$

- Onsager's principle (MDP) with incompressibility of flow, $\nabla \cdot \vec{u} = 0$ implies

$$\frac{1}{2} \frac{\delta \Delta}{\delta \vec{u}} \Big|_{\varepsilon=0} = - \int \left\{ \mu \Delta \vec{u} - \frac{\lambda}{\gamma} (\phi_t + \vec{u} \cdot \nabla \phi) \nabla \phi \right\} \cdot \vec{v} d\vec{x} = 0. \quad (23)$$

- Immiscible Two-phase Flow:

- The resulting system obtained by LAP and MDP with the manipulation on the dissipation is

$$\vec{u}_t + \vec{u} \cdot \nabla \vec{u} + \nabla p = \mu \Delta \vec{u} - \frac{\lambda}{\gamma} (\phi_t + \vec{u} \cdot \nabla \phi) \nabla \phi \quad (24)$$

$$\nabla \cdot \vec{u} = 0 \quad (25)$$

$$\phi_t + \vec{u} \cdot \nabla \phi = \gamma \left(\Delta \phi - \frac{1}{\eta^2} (\phi^2 - 1) \phi \right). \quad (26)$$

- The dissipative energy law:

$$\begin{aligned} & \frac{d}{dt} \int \left\{ \frac{1}{2} |\vec{u}|^2 + \lambda \left(\frac{1}{2} |\nabla \phi|^2 + \frac{1}{4\eta^2} (\phi^2 - 1)^2 \right) \right\} d\vec{x} \\ & = - \int \left(\mu |\nabla \vec{u}|^2 + \frac{\lambda}{\gamma} |\phi_t + \vec{u} \cdot \nabla \phi|^2 \right) d\vec{x}. \end{aligned} \quad (27)$$

- Remark:

- The dissipative force term in (24),

$$-\frac{\lambda}{\gamma}(\phi_t + \vec{u} \cdot \nabla \phi) \nabla \phi$$

is exactly same as the conservative force in (18),

$$\nabla \cdot (\nabla \phi \otimes \nabla \phi - W(\phi, \nabla \phi) I)$$

- As $\eta \rightarrow 0$, this is exactly the surface tension force on the interface³

³X.F. YANG, J.J. FENG, C. LIU, AND J. SHEN, *Numerical Simulations of Jet Pinching-off and Drop Formation Using An Energetic Variational Phase-Field Method*, J. Comput. Phys., 218(2006), pp.417–428.

- Immiscible Two-phase Flow (continue):
 - Computational Viewpoints:

$$\begin{aligned} \frac{d}{dt} \int \left\{ \frac{1}{2} |\vec{u}|^2 + \lambda \left(\frac{1}{2} |\nabla \phi|^2 + \frac{1}{4\eta^2} (\phi^2 - 1)^2 \right) \right\} d\vec{x} \\ = - \int \left(\mu |\nabla \vec{u}|^2 + \frac{\lambda}{\gamma} |\phi_t + \vec{u} \cdot \nabla \phi|^2 \right) d\vec{x}. \end{aligned} \quad (28)$$

: Lower Order Approximation in Numerical Simulations

$$\begin{aligned} \frac{d}{dt} \int \left\{ \frac{1}{2} |\vec{u}|^2 + \lambda \left(\frac{1}{2} |\nabla \phi|^2 + \frac{1}{4\eta^2} (\phi^2 - 1)^2 \right) \right\} d\vec{x} \\ = - \int \left(\mu |\nabla \vec{u}|^2 + \lambda \gamma |\Delta \phi - \frac{1}{\eta^2} (\phi^2 - 1) \phi|^2 \right) d\vec{x}. \end{aligned} \quad (29)$$

: High Order Approximation in Numerical Simulations

- **Another Example:** an incompressible viscoelastic complex fluid model⁴ with the elastic energy, $W(F) = \frac{1}{2}|F|^2$

- The energy law:

$$\frac{d}{dt} \int \left(\frac{1}{2} |\vec{u}|^2 + \frac{1}{2} |F|^2 \right) d\vec{x} = - \int \mu |\nabla \vec{u}|^2 d\vec{x}. \quad (30)$$

- The system of equations satisfies the energy law (30):

$$\vec{u}_t + \vec{u} \cdot \nabla \vec{u} + \nabla p = \mu \Delta \vec{u} + \nabla \cdot (W_F F^{-T}) \quad (31)$$

$$\nabla \cdot \vec{u} = 0 \quad (32)$$

$$F_t + \vec{u} \cdot \nabla F = \nabla \vec{u} F \quad (33)$$

: $W_F F^{-T}$ is conservative force.

⁴F.H. LIN, C. LIU, AND P. ZHANG, *On Hydrodynamics of Viscoelastic Fluids*, Comm. Pure Appl. Math., LVIII(2005), pp. 1-35

- Another Example (continue): Add an artificial term ΔF into (33)

$$F_t + \vec{u} \cdot \nabla F = \nabla \vec{u} F + \varepsilon^2 \Delta F. \quad (34)$$

- The energy law of the system (31), (32), (34):

$$\frac{d}{dt} \int \left(\frac{1}{2} |\vec{u}|^2 + \frac{1}{2} |F|^2 \right) d\vec{x} = - \int (\mu |\nabla \vec{u}|^2 + \varepsilon^2 |\nabla F|^2) d\vec{x}. \quad (35)$$

- Apply MDP: the resulting energy equation is

$$\begin{aligned} \frac{d}{dt} \int \left(\frac{1}{2} |\vec{u}|^2 + \frac{1}{2} |F|^2 \right) d\vec{x} \\ = - \int (\mu |\nabla \vec{u}|^2 + \varepsilon^2 \mathcal{R}[F_t + \vec{u} \cdot \nabla F - \nabla \vec{u} F]^2) d\vec{x}. \end{aligned} \quad (36)$$

$W_F F^{-T}$ can also be derived from MDP.

- Finite Element Space :

$$\vec{u}_h \in \mathbf{V}_h = (P_1 \oplus \text{bubble})^2 \quad (37)$$

$$p_h \in W_h = P_1 \quad (38)$$

$$\phi_h \in Q_h = P_1 \quad (39)$$

for the finite dimensional solution pair (\vec{u}_h, p_h, ϕ_h) .

- Numerical Method : The explicit-implicit scheme⁵

$$\begin{aligned}
 & (\tilde{u}_{h,t}^{n+1}, \vec{v}_h) + \left(\left(\frac{3\vec{u}_h^n - \vec{u}_h^{n-1}}{2} \cdot \nabla \right) \vec{u}_h^{\frac{n+1}{2}}, \vec{v}_h \right) + \left(\frac{1}{2} \left(\nabla \cdot \frac{3\vec{u}_h^n - \vec{u}_h^{n-1}}{2} \right) \vec{u}_h^{\frac{n+1}{2}}, \vec{v}_h \right) \\
 & - (p_h^{\frac{n+1}{2}}, \nabla \cdot \vec{v}_h) = -(\mu \nabla \vec{u}_h^{\frac{n+1}{2}}, \nabla \vec{v}_h) - \frac{\lambda}{\gamma} \left(\tilde{\phi}_{h,t}^{n+1} \nabla \left(\frac{3\phi_h^n - \phi_h^{n-1}}{2} \right), \vec{v}_h \right) \quad (40)
 \end{aligned}$$

$$-\frac{\lambda}{\gamma} \left(\vec{u}_h^{\frac{n+1}{2}}, \nabla \left(\frac{3\phi_h^n - \phi_h^{n-1}}{2} \right) \right) \left(\nabla \left(\frac{3\phi_h^n - \phi_h^{n-1}}{2} \right), \vec{v}_h \right) \quad \text{for all } \vec{v}_h \in \mathbf{V}_h,$$

$$\left(\nabla \cdot \vec{u}_h^{\frac{n+1}{2}}, w_h \right) + \varepsilon (p_h^{\frac{n+1}{2}}, w_h) = 0 \quad \text{for all } w_h \in W_h, \quad (41)$$

$$\begin{aligned}
 & (\tilde{\phi}_{h,t}^{n+1}, q_h) + \left(\vec{u}_h^{\frac{n+1}{2}}, \left(\frac{3\phi_h^n - \phi_h^{n-1}}{2} \right) q_h \right) \\
 & = -\gamma \left(\nabla \phi_h^{\frac{n+1}{2}}, \nabla q_h \right) - \frac{\gamma}{\eta^2} (f_h(\phi_h^n, \phi_h^{n+1}), q_h) \quad \text{for all } q_h \in Q_h \quad (42)
 \end{aligned}$$

⁵P. Lin, and C. Liu, *Simulation of Singularity Dynamics in Liquid Crystal Flows: a C⁰ Finite Element Approach*, J. Comput. Phys., **215**(1) (2006), 348–362. .

where

$$f_h(\phi_h^n, \phi_h^{n+1}) = \left\{ \frac{(|\phi_h^{n+1}|^2 - 1) + (|\phi_h^n|^2 - 1)}{2} \right\} \phi_h^{\frac{n+1}{2}},$$

$$\tilde{u}_{h,t}^{n+1} = \frac{\vec{u}_h^{n+1} - \vec{u}_h^n}{\Delta t}, \quad \vec{u}_h^{\frac{n+1}{2}} = \frac{\vec{u}_h^{n+1} + \vec{u}_h^n}{2}, \quad \tilde{\phi}_{h,t}^{n+1} = \frac{\phi_h^{n+1} - \phi_h^n}{\Delta t}, \quad \phi_h^{\frac{n+1}{2}} = \frac{\phi_h^{n+1} + \phi_h^n}{2},$$

(\cdot, \cdot) is the inner product operator, and Δt is the time step for simulations and ε is a small positive constant, $0 < \varepsilon \ll 1$.

The scheme satisfies the energy dissipation law:

$$\left[\int \left\{ \frac{1}{2} |\vec{u}_h^{n+1}|^2 + \lambda \left(\frac{1}{2} |\nabla \phi_h^{n+1}|^2 + \frac{1}{4\eta^2} |\phi_h^{n+1} - 1|^2 \right) \right\} d\vec{x} \right]_{h,t} =$$

$$- \int \left\{ \mu |\nabla \vec{u}_h^{n+1}|^2 + \varepsilon |\phi_h^{\frac{n+1}{2}}|^2 + \frac{\lambda}{\gamma} \left| \tilde{\phi}_{h,t}^{n+1} + (\vec{u}_h^{\frac{n+1}{2}} \cdot \nabla) \left(\frac{3\phi_h^n - \phi_h^{n-1}}{2} \right) \right|^2 \right\} d\vec{x}. \quad (43)$$

- Simulation 1 - Initial Data :

$$\vec{u}_0 = \vec{0}, \quad \phi_0 = \tanh\left(\frac{d_1(x, y)}{\eta\sqrt{2}}\right) + \tanh\left(\frac{d_2(x, y)}{\eta\sqrt{2}}\right) - 1.0 \quad (44)$$

with

$$d_1(x, y) = \sqrt{(x - 0.38)^2 + (y - 0.5)^2} - 0.11,$$

$$d_2(x, y) = \sqrt{(x - 0.62)^2 + (y - 0.5)^2} - 0.11,$$

$$\mu = 1.0, \quad \eta = 0.01, \quad \lambda = 0.01.$$

- Simulation 1.- Initial Data, ϕ_0 :

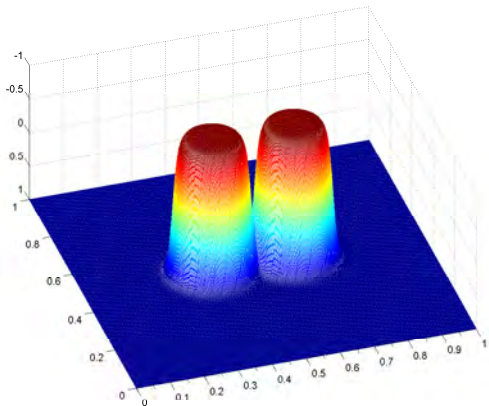


Figure: Initial Phase Field for Simulation.

Numerical Simulations

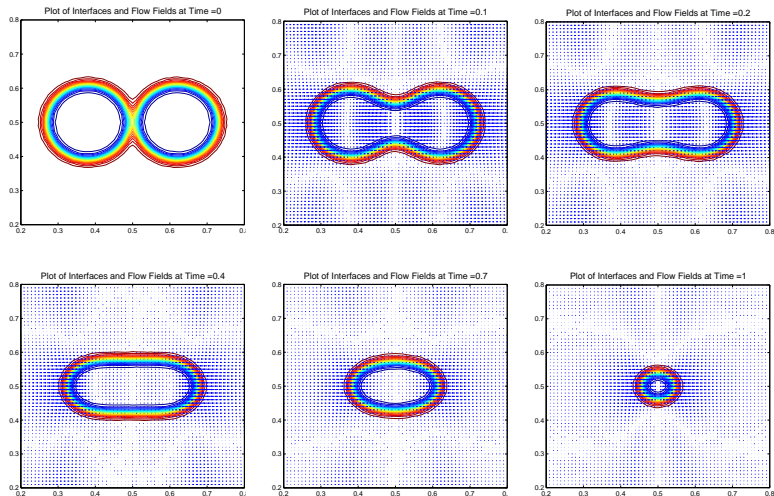


Figure: The time evolution results (merging effect) of phase field and velocity field from left to right and top to bottom ($t = 0.0, 0.1, 0.2, 0.4, 0.7, 1.0$ and $\Delta t = 0.001$).

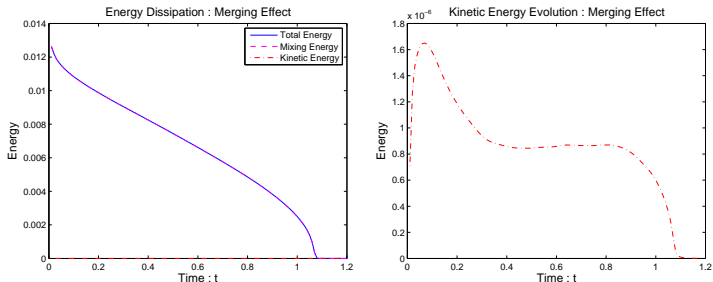


Figure: The total energy dissipation (left) and the kinetic energy (right) of merging phenomena in two-phase interface model.

- Simulation 2 - Initial Data :

$$\vec{u}_0 = \vec{0}, \quad \phi_0 = \tanh\left(\frac{d_1(x, y)}{\eta\sqrt{2}}\right) + \tanh\left(\frac{d_2(x, y)}{\eta\sqrt{2}}\right) - 1.0 \quad (45)$$

with

$$d_1(x, y) = \sqrt{(x - 0.38)^2 + (y - 0.38)^2} - 0.22,$$

$$d_2(x, y) = \sqrt{(x - 0.70)^2 + (y - 0.70)^2} - 0.08,$$

$$\mu = 1.0, \quad \eta = 0.01, \quad \lambda = 0.01.$$

- Simulation 2.- Initial Data, ϕ_0 :

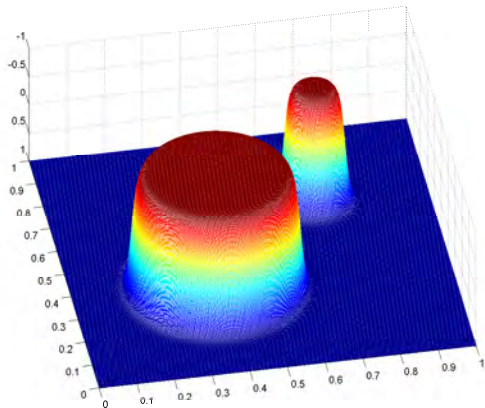


Figure: Initial Phase Field for Simulation.

Numerical Simulations

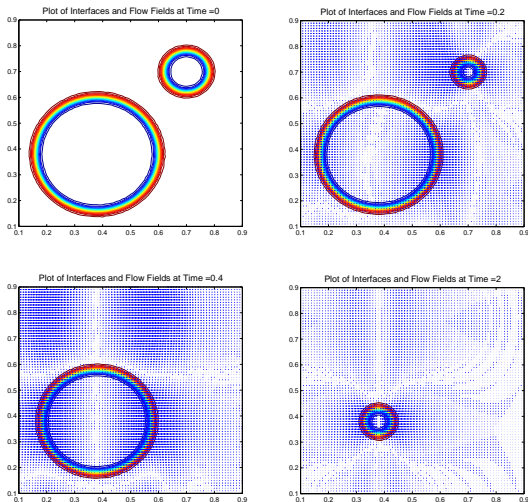


Figure: The time evolution results of phase field and velocity field from left to right and top to bottom ($t = 0.0, 0.2, 0.4, 2.0$ and $\Delta t = 0.001$).

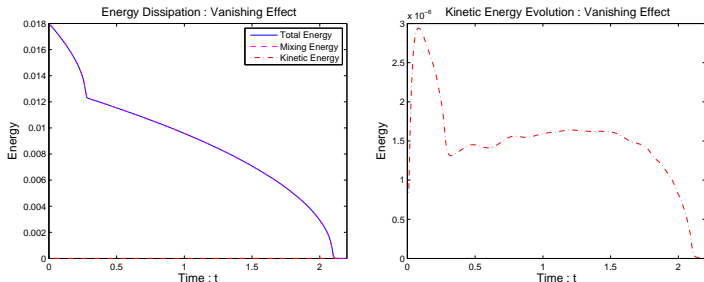


Figure: The total energy dissipation (left) and the kinetic energy (right) of vanishing phenomena in two-phase interface model.

- LAP : Conservative Force
- MDP : Dissipative Force
- MDP : Whether the dissipation functional includes the “rate” functions in time t of all “variables”
- The conservative force in hydrodynamic system is consistent with the dissipative force
- MDP plays an important role in designing numerical algorithms to solve the hydrodynamic complex fluid problem
- Difficulty : The optimal order of convergence for the finite element space

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Thank You!