Model reduction for two-phase flow problems by the Onsager variational principle

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1. The Onsager variational principle
2. Modelling by the Onsager principle
3. Approximations based on the Onsager principle

Lars Onsager

- November 27, 1903-October 5, 1976
- A Norwegian-born American physical chemist and theoretical physicist
- The Gibbs Professor at Yale University
- He was awarded the Nobel Prize in Chemistry in 1968
- Work: Thermodynamics is about heat and its conversion into other forms of energy - basically involving statistical descriptions of atomic and molecular movements. Irreversible thermodynamic processes go in only one direction and not in the reverse. Lars Onsager analyzed mathematical equations for various irreversible thermodynamic processes and in 1931 found the connection that led him to formulate equations that came to be known as reciprocal relations. This allowed a complete description of irreversible processes.

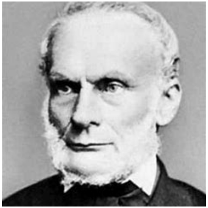
Thermodynamic equilibrium

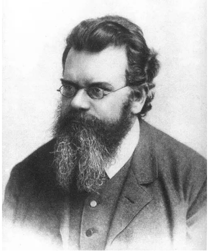
- When a closed system has been placed in contact with a heat reservoir for sufficient long time
- or when a large isolated thermodynamic system is left alone for sufficient long time

it will come to thermodynamic equilibrium.

- The macroscopic properties do not change.
- The microscopic states change all the time.
- Macroscopic quantities are “averages” of microscopic ones.

Entropy





- Boltzmann relation:

$$S = k_B \ln \Omega + const$$

- It is discovered by R. Clausius. L. Boltzmann set its statistics foundation.

$$dS = \frac{\delta Q}{T} \quad \text{(for reversible processes)}$$

Irreversible processes

- Irreversible thermodynamic processes go in only one direction and not in the reverse.
- Locally near equilibrium assumption
- Fluxes in irreversible processes

Principle of increase of entropy

- Principle of increase of entropy:
  If an isolated system is not in equilibrium state, the entropy will increase in the process it relaxes to the equilibrium state.

$$dS > 0.$$

- Helmholtz free energy:

$$E = U - TS.$$

- For isothermal systems: $dE < 0$.
- Energy changing rate

$$\dot{E} = \sum_i J_i \cdot F_i$$

Linear response regime

- Linear relation between general forces and general fluxes
- Examples

$$
\begin{aligned}
\text{Fourier's law:} \qquad & J_q = -k\nabla T, \qquad \text{(thermal flux)} \\
& \quad k : \text{thermal conductivity;} \\
\text{Fick's law:} \qquad & J_\phi = -D\nabla \phi, \qquad \text{(partical flux)} \\
& \quad D : \text{diffusion coefficient;} \\
\text{Ohm's law:} \qquad & J_e = -\sigma\nabla U, \qquad \text{(electric flux)} \\
& \quad \sigma : \text{electic conductivity.}
\end{aligned}
$$

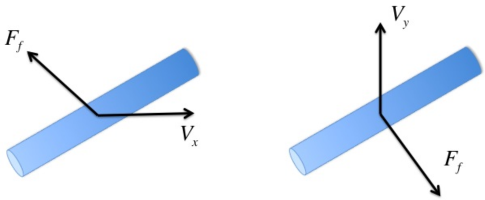
Reciprocal relation in multi-physics processes

- W. Thomson(Load Kelvin) did experiments for thermoelectricity. Let J_1 and J_2 be the thermal flux and electric flux, respectively. Then he discovered the relation

$$\begin{cases} F_1 = R_{11} J_1 + R_{12} J_2, \\ F_2 = R_{21} J_1 + R_{22} J_2, \end{cases}$$

  and the friction coefficients satisfy $R_{12} = R_{21}$.
- Helmholtz discovered similar relation for mixture of gases or liquid solutions.
- Lorentz studied the viscous fluids and found the reciprocal relation between the general velocity and general friction force. This is called Lorentz reciprocal relations.
- L. Onsager proved the reciprocal relation that for general systems.

The Lorentz reciprocal relation



- A rigid body moving in a viscous liquid with a constant velocity $\mathbf{v}$
- The friction forces $\mathbf{F}_{fri}$
- The linear relation

$$\mathbf{F}_{fri} = -R\mathbf{v}, \tag{1}$$

- The Lorentz reciprocal relation

$$R = R^T$$

In the above example, $F_{fy}/V_x = F_{fx}/V_y$.

Onsager reciprocal relations in irreversible process

- Reciprocal relation: Suppose that "flux" $\dot{x}_i$ and "forces" F_i are in linear response regime $\dot{x}_i = L_{ij} F_j$, then

$$L_{ij} = L_{ji}. \tag{2}$$

- A fundamental law in thermodynamics: diffusion, thermoelectricity, piezoelectric, ...

L. Onsager, Reciprocal relation in irreversible process I, Physical Review, 1931

L. Onsager, Reciprocal relation in irreversible process II, Physical Review, 1931

Onsager's proof for the Reciprocal relations

- Local equilibrium:
  $< x_i - x_i^0 >= 0, < \Delta x_i(-t)\Delta x_j(0) >=< \Delta x_i(0)\Delta x_j(t) >$.
- Microscopic time reversibility:
  $< \Delta x_i(t)\Delta x_j(0) >=< \Delta x_i(-t)\Delta x_j(0) >$
- Then one derive: $< \Delta x_i(t)\Delta x_j >=< \Delta x_i(0)\Delta x_j(t) >$.
- the Langevin equation

$$-\sum_j \zeta_{ij}\dot{x}_j - \frac{\partial A}{\partial x_i} + F_{ri}(t) = 0.$$

- Using $< F_{ri}(t) >= 0$, one can prove that $\zeta_{ij} = \zeta_{ji}$.

L. Onsager, Reciprocal relation in irreversible process II, Physical Review, 1931

M. Doi, Soft matter physics, Oxford University Press, 2014

The Onsager principle

- Let $x = (x_1, x_2, \cdots, x_f)$ represents a set of parameters which specify the non-equilibrium state of a system. It satisfies:

$$\sum_j \zeta_{ij}(x)\dot{x}_j = -\frac{\partial A}{\partial x_i}$$

where $A(x)$ is the free energy.

- Onsager's reciprocal relation:

$$\zeta_{ij} = \zeta_{ji}$$

- The equation can be derived by minimizing the Rayleighian:

$$R(x, \dot{x}) = \frac{1}{2}\sum_{i,j} \zeta_{ij}\dot{x}_i\dot{x}_j + \sum_i \frac{\partial A}{\partial x_i}\dot{x}_i$$

with respect to $\dot{x}_i$.

- $\Phi = \frac{1}{2}\sum_{i,j}\zeta_{ij}\dot{x}_i\dot{x}_j$ is the energy dissipation function(defined as a half of the energy dissipated per unit time)

L. Onsager, Reciprocal relation in irreversible process I, Physical Review, 1931
L. Onsager, Reciprocal relation in irreversible process II, Physical Review, 1931,
M. Doi, Soft matter physics, Oxford University Press, 2014

Related variational methods

- GENERIC approach, H. C. Ottinger
- Energetic variational method, Chun Liu
- Generalized Onsager principle, Qi Wang
- ...

- The variational principle has been used to derive many models in soft matter, like diffusion, complex fluids, liquid crystal, gel, etc.

Derivation of the diffusion equation

- The free energy

$$E = \int_\Omega k_B T \phi \ln \phi - \phi U(x) dx$$

- Transport equation

$$\frac{\partial \phi}{\partial t} + \mathrm{div}(\phi v) = 0.$$

- The energy dissipations

$$\Phi = \int_\Omega \frac{\xi}{2} \phi v^2 dx.$$

Derivation of the diffusion equation:Continued

- The Rayleighean

$$\mathcal{R} = \dot{E} + \Phi$$

- Minimization of the Rayleighean with respect to v.

$$\min_{v} \mathcal{R}(v)$$

- The Euler-Lagrange equation

$$v = -\frac{1}{\xi\phi}\nabla\phi + \frac{1}{\xi}\nabla U$$

- The diffusion equation

$$\frac{\partial\phi}{\partial t} - D\Delta\phi + \xi^{-1}\,\mathrm{div}\,(\phi\nabla U) = 0.$$

where $D = \frac{k_B T}{\xi}$.

Derivation of the Stokes Equation

- $\Phi = \frac{\eta}{2}\int_\Omega (\partial_i v_j + \partial_j v_i)^2 dx$, $A = \int_\Omega \rho g x_3 dx$
- Constraint: $\mathrm{div}\,\mathbf{v} = 0.$
- Using Onsager principle,

$$\min R = \Phi + \dot{A}$$
$$s.t.\, \mathrm{div}\,\mathbf{v} = 0.$$

- The Stokes equation

$$-\eta\Delta\mathbf{v} + \nabla p = -\rho g \mathbf{e}_3,$$
$$\mathrm{div}\,\mathbf{v} = 0.$$

- Onsager principle is used to derive the boundary condition for the contact lines.(GNBC)

T. Qian, X. Wang, P. Sheng, J. Fluid Mech. 2015.

A dynamic Allen-Cahn equation for wetting phenomena

- The phase-field approximation for interface energies

$$\mathcal{E}_\varepsilon(\phi) = \int_\Omega \frac{\varepsilon}{2}|\nabla\phi|^2 + \frac{1}{\varepsilon} f(\phi)\mathrm{d}x + \int_\Gamma g(\phi)\mathrm{d}s, \tag{3}$$

where $f(\phi_\varepsilon) = \frac{(1-\phi_\varepsilon^2)^2}{4}$ and $g(\phi_\varepsilon) = -\frac{\sigma}{4}\cos\theta_Y(s)(3\phi_\varepsilon - \phi_\varepsilon^3)$ with $\sigma = \frac{2\sqrt{2}}{3}$.

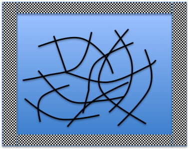
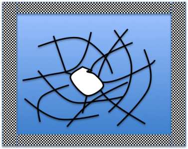
- The energy dissipation

$$\Phi = \frac{1}{2}\int_\Omega \dot{\phi}^2\mathrm{d}x + \frac{\xi}{2}\int_\Gamma \dot{\phi}^2\mathrm{d}s. \tag{4}$$

- Constraint $\int_\Omega \phi\mathrm{d}x = C_1$.
- Using the Onsager principle, we can derive

$$\begin{cases} \partial_t\phi - \varepsilon\Delta\phi + \varepsilon^{-1}f'(\phi) = \lambda, & \text{in } \Omega; \\ \xi\partial_t\phi + \varepsilon\partial_n\phi + g'(\phi) = 0, & \text{on } \Gamma; \\ \partial_n\phi = 0, & \text{on } \partial\Omega\setminus\Gamma; \\ \int_\Omega \phi dx = C_1. \end{cases} \tag{5}$$

Derivation of Gel dynamics

- The total energy

$$A = \int_{\Omega} W(\nabla \mathbf{u}) dx$$

- The energy dissipation

$$\Phi = \frac{\xi}{2} \int_{\Omega} (\dot{\mathbf{u}} - \mathbf{v}_s)^2 dx$$

- The constraint $\nabla \cdot (\phi \dot{\mathbf{u}} + (1 - \phi)\mathbf{v}_s) = 0.$

Dynamical Gel Model

- By using Onsager Principle,

$$\begin{aligned} &\min \dot{A} + \Phi \\ &s.t.\ \nabla \cdot (\phi \dot{\mathbf{u}} + (1-\phi)\mathbf{v}_s) = 0. \end{aligned}$$

- The dynamic equation:

$$\begin{aligned} &\xi(\dot{\mathbf{u}} - \mathbf{v}_s) - \mathrm{div}\Big[\frac{\partial W(\nabla \mathbf{u})}{\partial F}\Big] - \phi \nabla p = 0, \\ &\xi(\dot{\mathbf{u}} - \mathbf{v}_s) + (1-\phi)\nabla p = 0, \\ &\nabla \cdot (\phi \dot{\mathbf{u}} + (1-\phi)\mathbf{v}_s) = 0, \end{aligned}$$

- Onsager principle can be used to derive dynamic equations for many problems in soft matter.

Model reduction based on the Onsager principle

- Let $a(t) = \{a_1(t), a_2(t), \cdots, a_N(t)\}$ be the set of slow variables in a complex system

- The motion of the system, i.e. the time derivative $\dot{a}(t)$ is determined by

$$\min R(\dot{a}, a) = \Phi(\dot{a}, a) + \sum_i \frac{\partial A}{\partial a_i} \dot{a}_i$$

  Here $A(a)$ is the potential energy of the system, $\Phi(\dot{a}, a)$ is the energy dissipation function(defined as a half of the minimum of the energy dissipated per unit time in the fluid when the boundary is changing at rate $\dot{a}$)

- The reduced system

$$\frac{\partial \Phi}{\partial \dot{a}_i} + \frac{\partial A}{\partial a_i} = 0. \tag{6}$$

- The reduced model can be much easier to compute and analyze than the original problem.

M. Doi, Chinese Phys. B, (2015).

Many applications

- Diffusion

  M. Doi, Chinese Phys. B, (2015)

- Two-phase flow

  X. Xu, Y. Di, M. Doi, Phys. Fluids (2016),
  S. Guo, X. Xu, el al, J. Fluid Mech.(2019)
  X. Xu, X.-P. Wang, Phys. Fluids (2020),
  S. Lu, X.-P. Xu, J. Comput. Phys. (2021), ...

- Soft matter

  X. Man, M. Doi, Phys. Rev. Letter (2016)

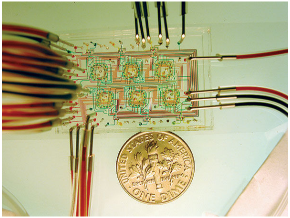
  J. Zhou, M. Doi, Phys. Rev. Fluids(2018),...

- Solid

  W. Jiang et al., Acta Mater. (2019).

  S. Dai, et al., CSIAM Tranc. Appl. Math. (2021)

Two-phase flow

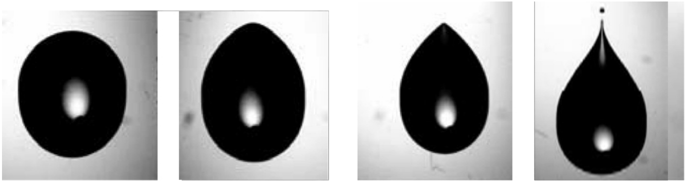


- Two-phase flow is a common in nature and in our daily life.

- Applications in microfluidics, coating, painting, printing, oil industry, etc.
- Many interesting physical problems involved

  contact line motion, contact angle hysteresis, Landau-Levich transition, droplet shape transitions, electrowetting

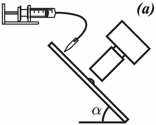
Sliding droplet on an inclined surface



- Sliding droplet problem has been studied both theoretically and experimentally.

  E. B. Dussan, JFM (1985,1987)
  L. Limat, et al, PRL (2001,2009), Phys. Fluid(2007), EPL (2004)

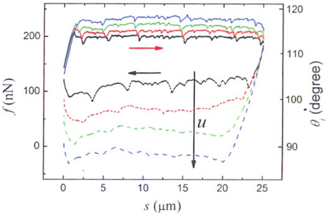
  M. B. Amar, L. J. Cummings, and Y. Pomeau, Phys. Fluid(2004) ...



- Theoretical analysis is elaborate

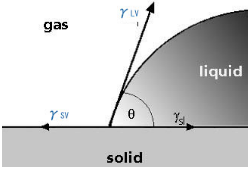
  It requires the asymptotic matching between the bulk solution and the solution near the contact line for the fluid equations

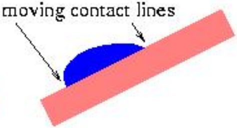
A recent experiment on contact angle hysteresis



- Experiments in *D. Guan, et al. PRL (2016)* show that there is an obvious contact angle hysteresis.
- Furthermore, the contact angle hysteresis is velocity dependent and might be asymmetric.

Two-phase flow with moving contact line: The modelling difficulties





- When the contact line moves, the standard no-slip boundary condition $\mathbf{u}|_{\partial\Omega} = 0$ leads to infinite energy dissipation

Huh, C. and Scriven, L., J. Colloid Interface Sci., 1971.
D. Bonn, J. Eggers, etc. Reviews of Modern Physics, 2009.
Snoeijer, J. and Andreotti, B., Annual review of fluid mechanics, 2013 .
Qian, T., Wang, X.-P. and Sheng, P., Phys. Rev. E 2003, J. Fluid Mech.,2006.
Ren, W., E, W., Phys. Fluids , 2011.

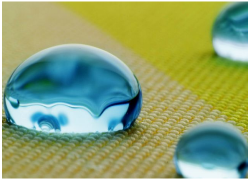
Boundary conditions for moving contact line

In literature, there are many different models

- Navier-slip BC: $v_\tau = -l_s \frac{\partial v_\tau}{\partial n}, \qquad \theta_d = \theta_Y$
- effective contact line velocity by uncompensated Young force
  $$v_{CL} = \gamma(\cos\theta_d - \cos\theta_Y)$$
- some effective models, e.g. $\theta_d = g(\theta_Y, v_\tau)$
- diffuse-interface models, e.g. GNBC

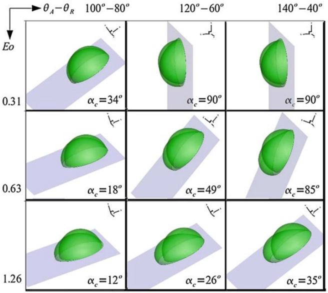
Cox, R., J. Fluid Mech., 1986.
Qian, T., Wang, X.-P. and Sheng, P., J. Fluid Mech.,2006.
Ren, W., E, W., Phys. Fluids , 2011.
Jacqmin, D., J. Fluid Mech. 2000.
Shikhmurzaev, Y., International J. Multiphase Flow, 1993...

A multi-scale free boundary problem



- MCL is a dynamic multiscale problem, the microscopic (nano scale) slip effect near the CL must be taken into account.
- Rough and inhomogeneous solid surfaces make the problem more complicated.

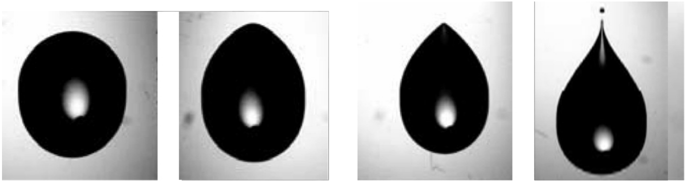
Numerical difficulties



- Solving two-phase Navier-Stokes equation with MCL conditions. GNBC(Qian, Wang, Sheng 2003), Ren, E(2017), etc.

  Require high level of numerical techniques and huge computational resources. For a 3D problem, a parallel computation is needed (M. Maglio, D. Legendre, 2014)

Sliding droplet on a inclined surface



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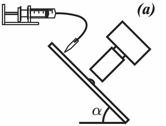
  L. Limat, et al, PRL (2001,2009), Phys. Fluid(2007), EPL (2004)

  M. B. Amar, L. J. Cummings, and Y. Pomeau, Phys. Fluid(2004) ...

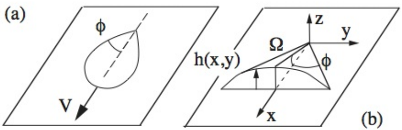


- Theoretical analysis is elaborate

  It requires the asymptotic matching between the bulk solution and the solution near the contact line for the fluid equations

- Numerical calculation by standard finite element method is challenging. (M. Maglio, D. Legendre, 2014)

The sliding droplet problem



- A liquid drop sliding on an inclined plane.

  We take an orthogonal coordinate on the inclined plane: z axis is normal to the substrate, y axis in the horizontal plane, x axis in downward direction.

- The shape of the droplet is given by $z = h(x, y, t)$. Assume:

$$h(x, y, t) = H(x, t)\left[1 - \left(\frac{y}{Y(x, t)}\right)^2\right].$$

$H(x, t)$ and $Y(x, t)$ have the following form:

$$H(x, t) = (x - a_1(t))(a_2(t) - x)(a_3(t) + a_4(t)x),$$
$$Y(x, t) = (x - a_1(t))^{\frac{1}{2}}(a_2(t) - x)^{\frac{1}{2}}(a_5(t) + a_6(t)x).$$

where $a_i(t)(i = 1, 2, ..., 6)$ are parameters to be determined by the variational principle.

- By volume conservation, only five parameters are independent.

Calculations of the potential energy and the energy dissipation

- The potential energy of the system is written as

$$A(a) = \int_{a_1}^{a_2} dx \int_{-Y}^{Y} dy \left[\frac{1}{2}\gamma\theta_e^2 + \frac{1}{2}\gamma[(\partial_x h)^2 + (\partial_y h)^2] + \frac{1}{2}\rho g h^2 \sin\alpha - \rho g x h \cos\alpha \right]$$

- By lubrication theory, the energy dissipation function is give by

$$\Phi[v_x, v_y] = \frac{1}{2} \int_{a_1}^{a_2} dx \int_{-Y}^{Y} dy \frac{3\eta}{h}(v_x^2 + v_y^2)$$

- The problem is to calculate the average velocity v_x, v_y

Calculations of the average velocity

- The average velocities v_x and v_y are not uniquely determined by the volume conservation equation

$$\dot{h} = -\partial_x(v_x h) - \partial_y(v_y h)$$

The equation is rewritten as

$$\left(1 - \frac{y^2}{Y^2}\right)\left(\dot{H} + \partial_x(v_x H) + H\partial_y v_y\right) + \frac{2Hy}{Y^3}(y\dot{Y} + yv_x\partial_x Y - Yv_y) = 0 \quad (7)$$

This constraint is satisfied if v_x and v_y satisfy

$$\dot{H} + \partial_x(v_x H) + H\partial_y v_y = 0, \qquad y\dot{Y} + yv_x\partial_x Y - Yv_y = 0. \quad (8)$$

A simple velocity field which satisfy the above equations is

$$v_x(x, y, t) = V(x, t), \quad v_y(x, y, t) = W(x, t)y \quad (9)$$

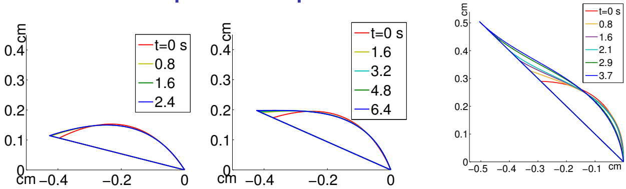
where $V(x, t)$ and $W(x, t)$ are given by

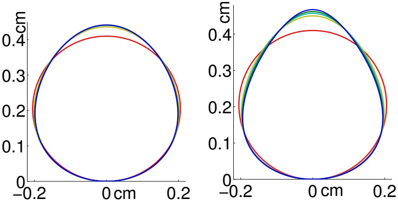
$$V(x, t) = -\frac{1}{HY}\int_{a_1}^{x}(\dot{H}Y + H\dot{Y})dx, \qquad W = \frac{1}{Y}\left(\dot{Y} + V\partial_x Y\right). \quad (10)$$

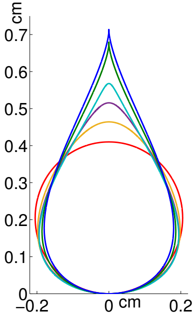
- The resulting system

$$\sum_{j=1}^{5}\zeta_{ij}\dot{a}_j + \frac{\partial A}{\partial a_i} = 0$$

Evolution of droplet shape on the inclined substrate



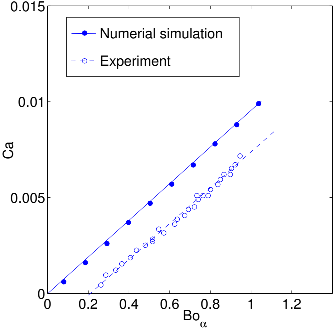




- Up : side view, Down: top view (Tilting angle: $15^o, 25^o, 45^o$)

X.Xu, Y. Di, M. Doi, Physics of Fluid (2016)

Capillary-Bond number relation

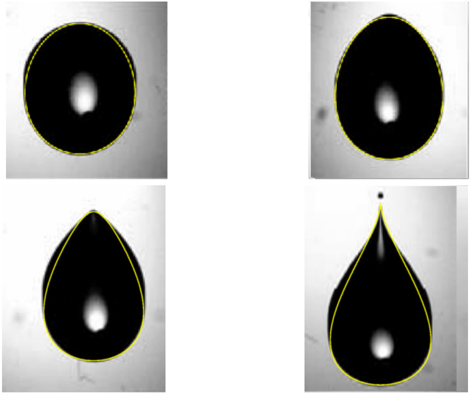


- Comparison with experimental results

  The sliding velocity U is represented by the capillary number $Ca = \eta U/\gamma$, and the inclination angle is represented by the bond number $Bo_\alpha = Bo \sin\alpha = V^{2/3}(\rho g/\gamma)\sin\alpha$.

- The discrepancy is due to the contact angle hysteresis.

Fitting experiments



- By adjusting the cut-off parameter, we can fit the shape of drops in experiments

The Allen-Cahn equation for wetting problem

- Consider the following problem

$$\begin{cases} \partial_t \phi - \varepsilon \Delta \phi + \varepsilon^{-1} f'(\phi) = \lambda, & \text{in } \Omega; \\ \xi \partial_t \phi + \varepsilon \partial_n \phi + g'(\phi) = 0, & \text{on } \Gamma; \\ \partial_n \phi = 0, & \text{on } \partial\Omega \setminus \Gamma; \\ \int_\Omega \phi dx = C_1. & \end{cases}$$

- It is extremely expansive to solve it on inhomogeneous or rough surfaces
  - Nonlinear boundary condition
  - ε must be much smaller than the roughness parameter

A simple method for mean curvature flow

Merriman, Bence, Osher (1992) introduce a threshold method for

$$\begin{cases} \phi_t - \varepsilon\Delta\phi + f'(\phi)/\varepsilon = 0, & \text{in } \Omega, \\ \partial_{\mathbf{n}}\phi = 0, & \text{on } \partial\Omega, \end{cases}$$

Operator splitting: In every time step:

- Solve a heat equation until δt:

$$\begin{cases} \phi_t - \varepsilon\Delta\phi = 0, & \text{in } \Omega, \\ \partial_{\mathbf{n}}\phi = 0, & \text{on } \partial\Omega, \end{cases}$$

- Solve the equation: $\phi_t + f'(\phi)/\varepsilon = 0, \text{in } \Omega$. When ε is small, by a very simple threshold technique

$$\phi(x) \approx \begin{cases} 1, & \text{if } \phi(x) > 0, \\ -1, & \text{if } \phi(x) < 0. \end{cases},$$

The threshold dynamics method

The threshold dynamic method has been used for mean curvature flow, multi-phase mean curvature flow, higher order geometric flows, etc.

- Develop of the method:

  Merriman, Bence, Osher (1992), S. Ruuth(1998),
  S. Esedoglu, S. Ruuth, R. Tsai (2010),

  S. Esedoglu and F. Otto(2015) ...

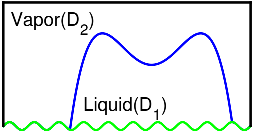
- Convergence analysis:

  L. C. Evans(1993), G. Barles, C. Georgelin (1995)
  K. Ishii (2005), A. Chambolle, M. Novaga(2006)

  T. Laux, F. Otto (2016), T. Laux, D. Swartz(2017)....

A MBO Method for wetting problem

$\Omega = D_1 \cup D_2$



Given two initial domain D_1, D_2 such that $|D_1| = V_0$.

- Solve a heat equation until δt:

$$\begin{cases} \phi_t - \varepsilon \Delta \phi = 0, & \text{in } \Omega, \\ \varepsilon \partial_{\mathbf{n}} \phi + \partial_\phi \gamma(\mathbf{x}, \phi) = 0, & \text{on } \Gamma_\varepsilon, \\ \phi(0) = \chi_{D_1}. \end{cases}$$

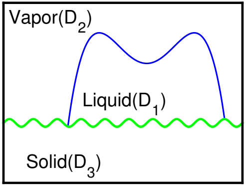
- A threshold step(redefine D_1): to find a δ, such that

$$D_1 = \{x : \phi(x) < 1/2 + \delta\} \qquad \text{and } |D_1| = V_0.$$

□ The heat equation is not easy to solve any more! Especially when the boundary is rough.

A threshold dynamics method based on extensions

$\tilde{\Omega} = D_1 \cup D_2 \cup D_3$



Step 1. For given set (D_1^k, D_2^k), we define two functions

$$\phi_1 = \frac{1}{\sqrt{\delta t}} G_{\delta t} * (\gamma_{LV} \chi_{D_2^k} + \gamma_{SL} \chi_{D_3}),\ \phi_2 = \frac{1}{\sqrt{\delta t}} G_{\delta t} * (\gamma_{LV} \chi_{D_1^k} + \gamma_{SV} \chi_{D_3}). \tag{11}$$

Step 2. Find a δ so that the set

$$\tilde{D}_1^\delta = \{x \in \Omega | \phi_1 < \phi_2 + \delta.\} \tag{12}$$

satisfies $|\tilde{D}_1^\delta| = V_0$. Denote $D_1^{k+1} = \tilde{D}_1^\delta$ and $D_2^{k+1} = \Omega \setminus D_1^{k+1}$.

X. Xu, D. Wang, X. Wang, J. Comput. Phys. (2017), D. Wang, X. Xu, X. Wang, J. Comput. Phys. (2018)

X. Xu, Y. Ying, Comm. Comput. Phys. (2021)

Numerical accuracy

Table : Accuracy check w.r.t the time step δt for the droplet spreading problem.

δt	L^1 Error	Convergence Rate	L^∞ Error	Convergence Rate
0.04	0.0676	–	0.0928	–
0.02	0.0347	0.95	0.0621	0.49
0.01	0.0170	1.04	0.0383	0.62
0.005	0.0079	1.14	0.0215	0.79

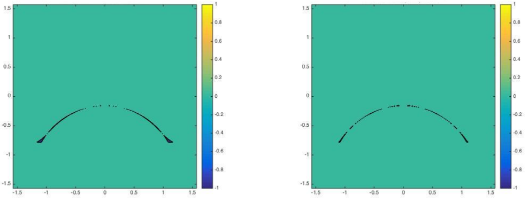


Figure : Left: without adaptivity in time, Right: with adpativity in time

- Half order accuracy with respect to δt
- A time refinement technique is developed

Reduced model for the Allen-Cahn equation

- Asymptotic expansions

$$\phi(x,t) = \phi_0(x,t) + \varepsilon\phi_1(x,t) + \cdots ,$$

where $\phi_0(x,t) = \tanh(\frac{d(x,t)}{\sqrt{2}\varepsilon})$ and $d(x,t)$ is a signed distance function.

- Approximated energy dissipations

$$\Phi \approx \frac{1}{\varepsilon^2}\int_\Omega f(\phi_0)(\partial_t d)^2 \mathrm{d}x + \frac{\xi}{\varepsilon^2}\int_\Gamma f(\phi_0)(\partial_t d)^2 \mathrm{d}s. \qquad (13)$$

- The approximate total free energy

$$\mathcal{E}_\varepsilon \approx \int_\Omega \frac{1}{\varepsilon} f(\phi_0)(|\nabla d(x,t)|^2 + 1)\mathrm{d}x + \int_\Gamma g(\phi_0)\mathrm{d}s. \qquad (14)$$

- By Onsager principle, we derive a linear equation for d

$$\begin{cases} \partial_t d - \varepsilon\Delta d = 0, & \text{in } \Omega; \\ \xi\partial_t d + \varepsilon(\partial_n d - \cos\theta_Y) = 0, & \text{on } \Gamma. \end{cases} \qquad (15)$$

A new diffusion generated method

- Solving a heat equation until δt

$$\begin{cases} \partial_t \varphi - \Delta \varphi = 0, & \text{in } \Omega; \\ \xi \partial_t \varphi + \partial_n \varphi = \cos \theta_Y, & \text{on } \Gamma; \\ \varphi(x, 0) = d_k(x). \end{cases} \tag{16}$$

- The re-distance of the function φ.

$$\nabla \tilde{d}_{k+1} = \frac{\nabla \varphi(x, \delta t)}{|\nabla \varphi(x, \delta t)|}$$

- Correction of the volume

$$d_{k+1}(x) = \tilde{d}_{k+1}(x) - \delta^*.$$

Numerical accuracy

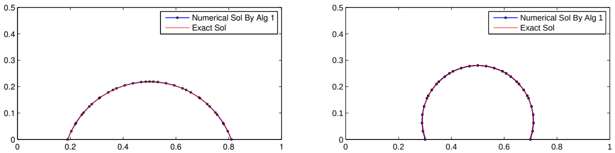


Figure : A comparison between the numerical solution obtained by Algorithm 1 and the exact solution.

Table : Numerical errors of Algorithm 1 for the case $\theta_Y = 110^o$

# Resolution	# $\delta t(t_{unit})$	# Error	# Order
8×8	1/2	9.96E-3	-
16×16	1/4	5.31E-3	0.91
32×32	1/8	2.68E-3	0.99
64×64	1/16	1.67E-3	0.68
128×128	1/32	7.42E-4	1.17

Stick-slip behaviour on a chemically patterned surface

Consider a droplet on an inhomogeneous surface. Increase its volume.

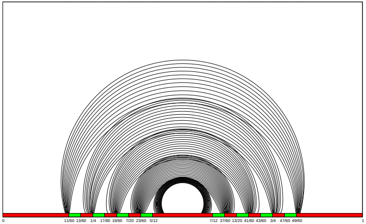


Figure : The drop profiles with increasing volume in the $k = 4$ case.

S. Lu, X. Xu, An efficient diffusion generated motion method for wetting dynamics, J. Comput. Phys.(2021)

Summary

- The Onsager principle can be a very powerful tool for model reduction.

- The reduced model captures the essential behaviour of slow variables.

- The Onsager principle can be used to derive efficient numerical schemes.

Ongoing work:

- Mathematical theory
- Numerical methods for multi-physics systems
- Other applications....

Thank you very much!