Integral Equation Method for Cahn-Hilliard Equation in Wetting Problems

Xiaoyu Wei[1]

[1]Department of Computer Science, University of Illinois at Urbana-Champaign

Feb 26, 2019

Joint work with Shidong Jiang[2], Andreas Klöckner[3] and Xao-Ping Wang[4]
(in alphabetical order)

[2]Department of Mathematical Sciences, New Jersey Institute of Technology
[3]Department of Computer Science, University of Illinois at Urbana-Champaign
[4]Department of Mathematics, the Hong Kong University of Science and Technology

Outline

Wetting Problem

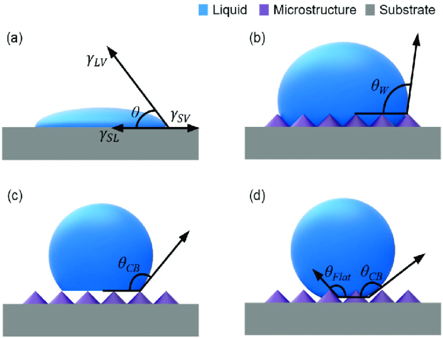
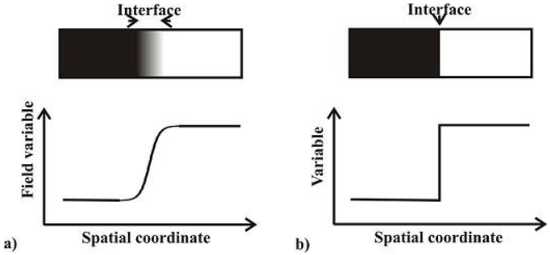


Figure: Illustration of droplet wetting on rough surfaces. Image from[1].

[1] Sahoo et al. 2018.

Phase-Field Modeling

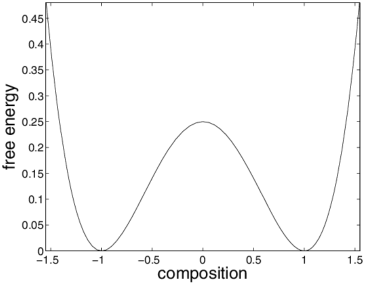
- *Smooth* "phase-field" function ϕ: -1 in liquid, 1 in vapor.
- *Small* interface "thickness" ϵ. (Image from the Internet[2]).



[2] *Nele Moelans' Website :: Research :: Phase Field Method* n.d.

Phase-Field Modeling (Cont'd)

- Total energy $\mathcal{E}_{tot} = \int_\Omega \mathcal{E}_{blk} + \int_{\partial\Omega} \gamma$.
- Ginzburg-Landau energy[3] $\mathcal{E}_{blk}[\phi] = \int_\Omega \frac{\epsilon}{2}\|\nabla\phi(\mathbf{x})\|^2 + \frac{[\phi(\mathbf{x})^2-1]^2}{4\epsilon} d\mathbf{x}$.



- Surface free energy $\gamma[\phi] = \frac{\sqrt{2}}{3}\cos\theta_Y \sin\left(\frac{\pi}{2}\phi\right)$.
- Equilibrium contact angle[4] (Young's angle) θ_Y.

[3] Cahn and Hilliard 1958.

[4] Xu and Wang 2010.

Modeling Equations

- Inside Ω,

$$\frac{\partial \phi(\mathbf{x}, t)}{\partial t} = \Delta \mu(\mathbf{x}, t) \tag{1}$$

$$\mu(\mathbf{x}, t) = -\epsilon \Delta \phi(\mathbf{x}, t) + \frac{\phi(\mathbf{x}, t)^3 - \phi(\mathbf{x}, t)}{\epsilon} \tag{2}$$

- On $\partial\Omega$,

$$\frac{\partial \phi(\mathbf{x}, t)}{\partial t} = -\epsilon \partial_n \phi(\mathbf{x}, t) + \frac{\partial \gamma(\phi)}{\partial \phi}(\mathbf{x}, t) \tag{3}$$

$$\partial_n \mu(\mathbf{x}, t) = 0 \tag{4}$$

where $\partial_n = \mathbf{n} \cdot \nabla$, and $\mathbf{n}$ is the unit outward normal of $\partial\Omega$.

Time Discretization

Convex splitting technique[5] is used for time discretization. In Ω,

$$\frac{\phi^{n+1}(\mathsf{x}) - \phi^n(\mathsf{x})}{\delta t} = \Delta\mu^{n+1}(\mathsf{x}),$$
$$\mu^{n+1}(\mathsf{x}) = -\epsilon\Delta\phi^{n+1}(\mathsf{x}) + \frac{s\phi^{n+1}(\mathsf{x}) - (1+s)\phi^n(\mathsf{x}) + (\phi^n)^3(\mathsf{x})}{\epsilon}$$

where s is a constant (more discussion later); and on the boundary,

$$\frac{\phi^{n+1}(\mathsf{x}) - \phi^n(\mathsf{x})}{\delta t} = -\epsilon\partial_n\phi^{n+1}(\mathsf{x}) + \frac{\partial\gamma}{\partial\phi}(\phi^n(\mathsf{x})),$$
$$\partial_n\mu^{n+1}(\mathsf{x}) = 0.$$

[5] Eyre 1997.

Discrete Energy Law

Convex splitting is energy stable regardless of time step size δt.

Theorem (Unconditional Stability)

If $|\phi^k(\mathbf{x})| \leq M, \forall k = 0, 1, \ldots, n$, and $s \geq (3M^2 - 1)/2$, the convex splitting scheme satisfies the following discrete energy law:

$$\mathcal{E}_{tot}^{n+1} - \mathcal{E}_{tot}^{n} \leq -\delta t(\nabla \mu^{n+1}, \nabla \mu^{n+1}).$$

Idea of the proof: convex splitting of energy $\mathcal{E}_{tot} = \mathcal{E}_c - \mathcal{E}_e$, with $\mathcal{E}_c$ convex, and the second variation of $\mathcal{E}_e$ bounded from below.
Recall:
$\mathcal{E}_{tot} = \int_\Omega \left(\frac{\epsilon}{2} \|\nabla \phi(\mathbf{x})\|^2 + \frac{[\phi(\mathbf{x})^2 - 1]^2}{4\epsilon} \right) d\mathbf{x} + \int_{\partial\Omega} \frac{\sqrt{2}}{3} \cos\theta_Y \sin\left(\frac{\pi}{2}\phi(\mathbf{x})\right) ds_{\mathbf{x}}$

Static BVPs

After time discretization, it remains to solve at each time step

$$(\Delta^2 - b\Delta + c)\phi^{n+1}(\mathbf{x}) = f_1(\mathbf{x}),$$
$$(\Delta - b)\phi^{n+1}(\mathbf{x}) + \frac{1}{\epsilon}\mu^{n+1}(\mathbf{x}) = f_2(\mathbf{x}),$$

subject to boundary conditions

$$(\partial_n + c)\phi^{n+1}(\mathbf{x}) = h(\mathbf{x}), \quad \frac{1}{\epsilon}\partial_n\mu^{n+1}(\mathbf{x}) = 0,$$

where $b = \frac{s}{\epsilon^2}$, $c = \frac{1}{\epsilon\delta t}$, and

$$f_1(\mathbf{x}) = c\phi^n(\mathbf{x}) - \frac{1+s}{\epsilon^2}\Delta\phi^n(\mathbf{x}) + \frac{1}{\epsilon^2}\Delta(\phi^n(\mathbf{x}))^3,$$
$$f_2(\mathbf{x}) = \frac{(\phi^n(\mathbf{x}))^3 - (1+s)\phi^n(\mathbf{x})}{\epsilon^2},$$
$$h(\mathbf{x}) = c\phi^n(\mathbf{x}) + \frac{1}{\epsilon}\frac{\partial\gamma}{\partial\phi}(\phi^n(\mathbf{x})).$$

Conversion to Pure BVP

Use volume potentials to eliminate the inhomogeneous terms by letting

$$\begin{aligned} \phi^{n+1}(\mathbf{x}) &= \tilde{u}(\mathbf{x}) + u(\mathbf{x}), & \tilde{u}(\mathbf{x}) &= V[\phi^n], \\ \frac{1}{\epsilon}\mu^{n+1}(\mathbf{x}) &= \tilde{v}(\mathbf{x}) + v(\mathbf{x}), & \tilde{v}(\mathbf{x}) &= f_2(\mathbf{x}) - (\Delta - b)\tilde{u}(\mathbf{x}), \end{aligned}$$

where $V[\phi^n]$ satisfies

$$(\Delta^2 - b\Delta + c)V[\phi^n](\mathbf{x}) = f_1(\mathbf{x}), \quad \forall \mathbf{x} \in \Omega.$$

Volume Potential

- One choice of $\tilde{u}$ is the volume potential

$$V_0[f_1] := \int_\Omega G_0(\mathbf{x}, \mathbf{y}) f_1(\mathbf{y}) d\mathbf{y},$$

where G_0 is the free-space Green's function s.t.,

$$(\Delta^2 - b\Delta + c) G_0(\mathbf{x}, \mathbf{y}) = \delta(\mathbf{x}, \mathbf{y}),$$

in the sense of distributions.

- To compute $\tilde{u}$: box-FMM + C^1 function extension.

Static Pure BVPs

u and v are the solutions to the following pure boundary value problem

$$
\begin{aligned}
(\Delta^2 - b\Delta + c)u(\mathbf{x}) &= 0, \\
v + (\Delta - b)u(\mathbf{x}) &= 0, \\
(\partial_n + c)u(\mathbf{x}) &= g_1(\mathbf{x}), \\
\partial_n v(\mathbf{x}) &= g_2(\mathbf{x}),
\end{aligned}
$$

where the boundary data g_1 and g_2 are given by

$$
\begin{aligned}
g_1(\mathbf{x}) &= h(\mathbf{x}) - \tilde{u}_n(\mathbf{x}) - c\tilde{u}(\mathbf{x}), \\
g_2(\mathbf{x}) &= -\tilde{v}_n(\mathbf{x}).
\end{aligned}
$$

Operator Factorization & Layer Potentials

- Factoring a quadratic polynomial:

$$x^2 - bx + c = (x - \lambda_1^2)(x - \lambda_2^2).$$

- Similarly, $\Delta^2 - b\Delta + c = (\Delta - \lambda_1^2)(\Delta - \lambda_2^2)$
- Denote G_i $(i = 1, 2)$ to be the free-space Green's function of the Yukawa operator $\Delta - \lambda_i^2$.
- Denote G_0 to be the free-space Green's function of the full operator $\Delta^2 - b\Delta + c$.
- Define layer potential operators S_i $(i = 0, 1, 2)$ as

$$S_i[\rho](\mathbf{x}) = \int_{\partial\Omega} G_i(\mathbf{x}, \mathbf{y})\rho(\mathbf{y})ds_{\mathbf{y}},$$

where $\rho(\mathbf{x}) \in L^2(\partial\Omega)$,

Solution Representation

- Represent u by the sum of two layer potentials

$$u(\mathbf{x}) = \int_{\partial\Omega} [G_1(\mathbf{x}, \mathbf{y})\sigma_1(\mathbf{y}) + G_0(\mathbf{x}, \mathbf{y})\sigma_2(\mathbf{y})] \, ds_{\mathbf{y}},$$

  where σ_i $(i = 1, 2)$ are the unknown densities on $\partial\Omega$.
- Plug in the equation to get representation of v

$$v(\mathbf{x}) = \int_{\partial\Omega} \left\{ \lambda_2^2 G_1(\mathbf{x}, \mathbf{y})\sigma_1(\mathbf{y}) + [\lambda_1^2 G_0(\mathbf{x}, \mathbf{y}) - G_1(\mathbf{x}, \mathbf{y})]\sigma_2(\mathbf{y}) \right\} ds_{\mathbf{y}}.$$

Second-Kind Integral Equation (SKIE) Formulation

- Plug representations of u, v into the boundary conditions to get boundary integral equations

$$(D + A)[\sigma](\mathbf{x}) = g(\mathbf{x}), \quad (\mathbf{x} \in \partial\Omega)$$

$$D = -\frac{1}{2}\begin{bmatrix} 1 & 0 \\ \lambda_2^2 & -1 \end{bmatrix}, \quad A = \begin{bmatrix} \partial_n S_1 + cS_1, & \partial_n S_0 + cS_0 \\ \lambda_2^2 \partial_n S_1, & -\partial_n S_1 + \lambda_1^2 \partial_n S_0 \end{bmatrix},$$

where $\sigma = [\sigma_1, \sigma_2]^T$, $g = [g_1, g_2]^T$.

- D has nonzero determinant, A is compact $\implies$ $D + A$ is a Fredholm integral equation of the second kind.
- To solve the SKIE: QBX + GMRES.

Fast Algorithms

- Box FMM (the Box Code)[6]
  - Volume potential evaluation in linear complexity
  - Efficient precompute-reuse strategy for the near-field.
  - Box-shaped geometry only.
- C^1 Function Extension[7]
  - Extend density from Ω to a bounding box.
  - Enables use of box FMM with non-box domains.
  - Exterior biharmonic extension with QBX + GMRES.
- Quadrature-by-Expansion (QBX)[8]
  - Layer potential evaluation
  - Evaluates layer potentials (singular quadrature).
  - Linear complexity when used with FMM.
  - Inplements `matvec` of the BIE.

[6] Ethridge and Greengard 2001.

[7] Rachh and Askham 2018.

[8] Klöckner et al. 2013.

Self-Convergence Test: 1st Order

Self-convergence test for one time step, first order discretization.

q_b	q_v	δx	e_0	Order
1	1	1.56×10^{-2}	9.55×10^{-1}	–
1	1	7.81×10^{-3}	4.55×10^{-1}	1.07
1	1	3.91×10^{-3}	1.24×10^{-1}	1.88
1	1	1.95×10^{-3}	6.66×10^{-2}	0.90
1	1	9.77×10^{-4}	3.09×10^{-2}	1.11
1	1	4.88×10^{-4}	1.04×10^{-2}	1.57

Table: Results Using First-Order Approximation.

Self-Convergence Test: 2nd Order

Self-convergence test for one time step, second order discretization.

q_b	q_v	δx	e_0	Order
2	4	1.56×10^{-2}	3.11×10^{-1}	–
2	4	7.81×10^{-3}	2.53×10^{-1}	0.30
2	4	3.91×10^{-3}	5.73×10^{-2}	2.14
2	4	1.95×10^{-3}	1.36×10^{-2}	2.07
2	4	9.77×10^{-4}	3.71×10^{-3}	1.87
2	4	4.88×10^{-4}	7.23×10^{-4}	2.36

Table: Results Using Second-Order Approximation.

Short-Time Dynamics: Problem Setup

- $\epsilon = 10^{-2}$, $\delta t = 10^{-4}$, $\theta_Y = \pi/3$.
- Initials are generated with B-spline interpolation, using
  1. a 200×200 Cartesian grid points as knots, and
  2. uniformly random nodal values in $[-10^{-3}, 10^{-3}]$.

  The idea here is to mimic a near-uniform state with random perturbations.

Short-Time Dynamics: Initial Condition

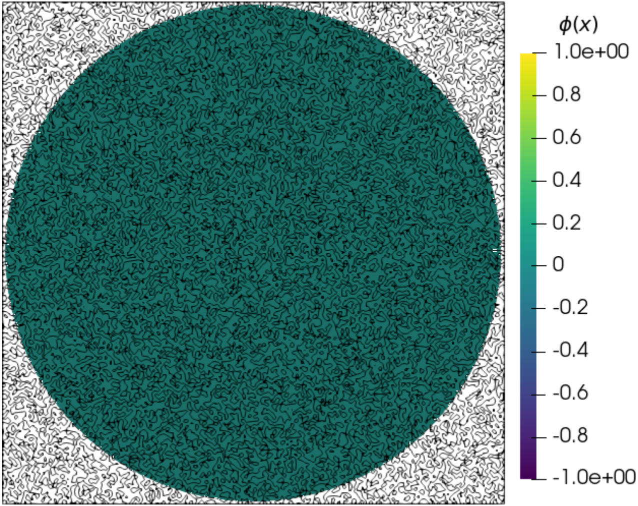
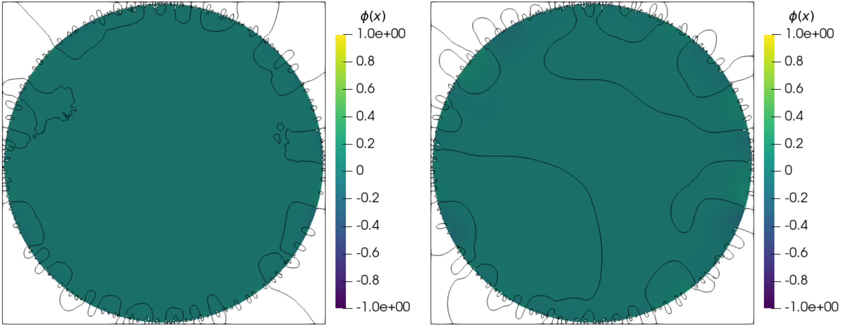


Figure: Initial Condition.

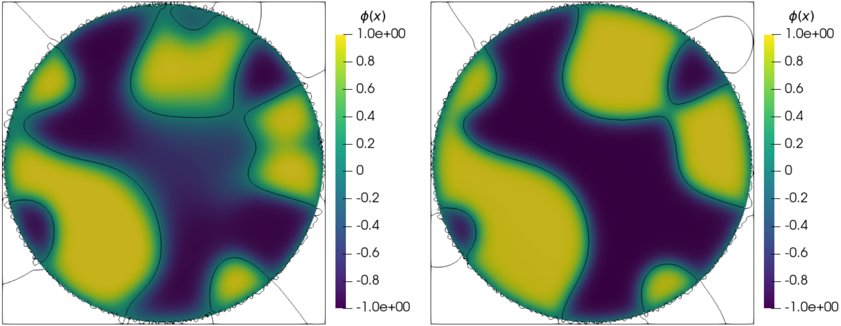
Short-Time Dynamics (Cont'd)



(a) $t = \delta t$. (b) $t = 5\delta t$.

Figure: Short-Time Dynamics.

Short-Time Dynamics (Cont'd)



(a) $t = 20\delta t$.   (b) $t = 30\delta t$.

Figure: Short-Time Dynamics.

Long-Time Dynamics: Problem Setup

- $\epsilon = 10^{-2}$, $\delta t = 0.5$, $\theta_Y = \pi/3$.
- Initial condition: $\phi^0(x, y) = \sin\left(\frac{40\pi}{L}x\right)\cos\left(\frac{32\pi}{L}y\right)$, where $L = 0.5$ is the size of the bounding box.

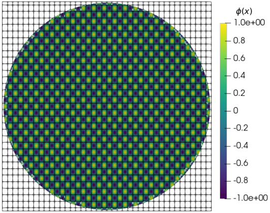
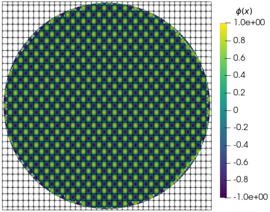


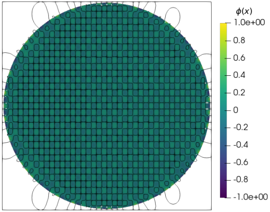
Figure: Initial Condition.

- Stabilized representation is used to workaround boundary layer issues.

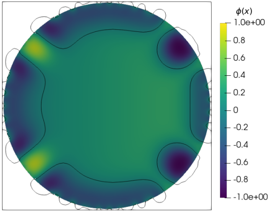
Long-Time Dynamics (Cont'd)



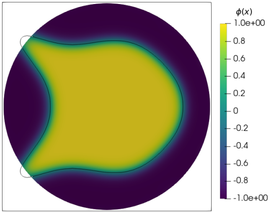
(a) $t = 0.$



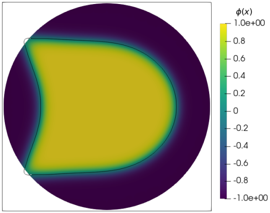
(b) $t = \delta t.$



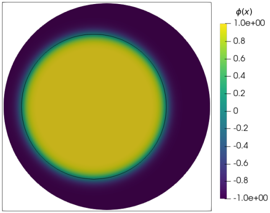
(c) $t = 11\delta t.$



(d) $t = 51\delta t.$



(e) $t = 101\delta t.$



(f) $t = 1451\delta t.$

2nd Order IEM vs 2nd Order Mixed-FEM

δx	$N_{DOFs}(FEM)$	$\kappa(FEM)$
1.11×10^{-1}	16	9.79×10^{3}
6.26×10^{-2}	50	1.24×10^{4}
3.32×10^{-2}	178	2.15×10^{4}
1.71×10^{-2}	674	6.82×10^{4}
8.64×10^{-3}	2626	1.12×10^{5}

δx	$N_{DOFs}(IEM)$	$\kappa(IEM)$
1.11×10^{-1}	28	9.86×10^{2}
6.26×10^{-2}	50	9.87×10^{2}
3.32×10^{-2}	100	9.88×10^{2}
1.71×10^{-2}	182	9.88×10^{2}
8.64×10^{-3}	360	9.89×10^{2}

Summary

- Integral equation method for the Cahn-Hilliard equation in bounded 2D domains with solid boundary conditions.
- Two stages for each time step:
  1. evaluate volume potentials and
  2. solve remaining SKIE.
- Advantages:
  1. Small number of unknowns.
  2. Well conditioned linear systems.
- Future Work
  1. Alternative methods to density extension approach.
  2. Generalization to 3D problems.
  3. QBX direct solver.

References I

Cahn, John W. and John E. Hilliard (Feb. 1958). "Free Energy of a Nonuniform System. I. Interfacial Free Energy". In: *The Journal of Chemical Physics* 28.2, pp. 258–267. ISSN: 0021-9606. DOI: 10.1063/1.1744102.

Ethridge, F. and L. Greengard (Jan. 2001). "A New Fast-Multipole Accelerated Poisson Solver in Two Dimensions". In: *SIAM Journal on Scientific Computing* 23.3, pp. 741–760. ISSN: 1064-8275. DOI: 10.1137/S1064827500369967.

Eyre, David J. (1997). *An Unconditionally Stable One-Step Scheme for Gradient Systems*.

Klöckner, Andreas et al. (Nov. 2013). "Quadrature by Expansion: A New Method for the Evaluation of Layer Potentials". In: *Journal of Computational Physics* 252, pp. 332–349. ISSN: 0021-9991. DOI: 10.1016/j.jcp.2013.06.027.

References II

Nele Moelans' Website :: Research :: Phase Field Method (n.d.). http://nele.studentenweb.org/research/?subject=PFM.

Rachh, Manas and Travis Askham (May 2018). "Integral Equation Formulation of the Biharmonic Dirichlet Problem". In: *Journal of Scientific Computing* 75.2, pp. 762–781. ISSN: 0885-7474, 1573-7691. DOI: 10.1007/s10915-017-0559-8. arXiv: 1705.09715.

Sahoo, Bichitra et al. (Feb. 2018). "Chemical and Physical Pathways for Fabricating Flexible Superamphiphobic Surfaces with High Transparency". en. In: *Coatings* 8.2, p. 47. DOI: 10.3390/coatings8020047.

References III

Xu, X. and X. Wang (Jan. 2010). "Derivation of the Wenzel and Cassie Equations from a Phase Field Model for Two Phase Flow on Rough Surface". In: *SIAM Journal on Applied Mathematics* 70.8, pp. 2929–2941. ISSN: 0036-1399. DOI: 10.1137/090775828.