Introduction to the Phase Field Method
Allen-Cahn vs. Cahn-Hilliard Model

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What for?

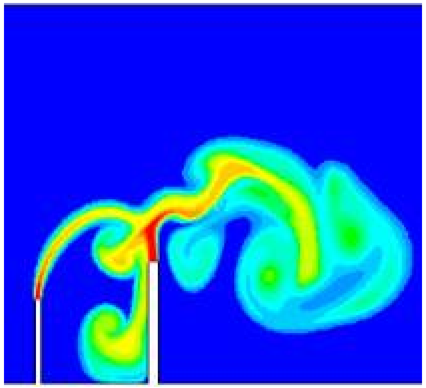
The phase-field method (PFM), as presented here, grows out of the work of *Cahn, Hilliard* and *Allen*

It is used for two general purposes:

- to model systems in which the diffuse nature of interfaces is essential to the problem, such as **spinodal decomposition** and **solute trapping** during rapid phase boundary motion;
- as a front tracking technique to model general **multi-phase systems**.

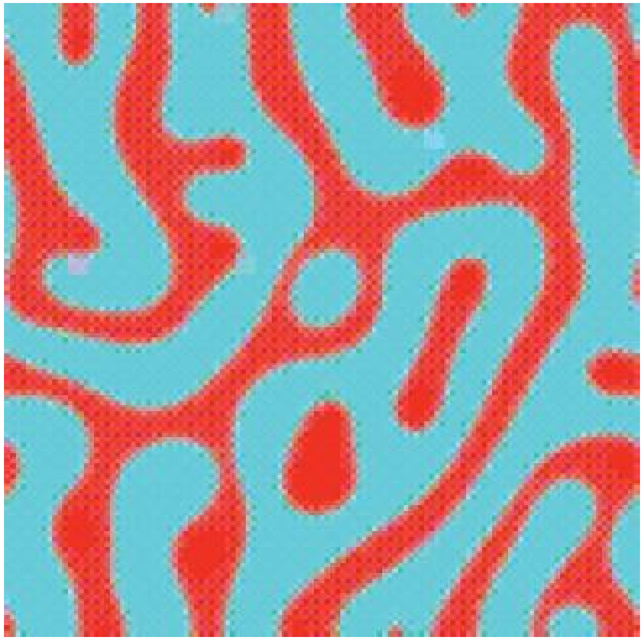
PFM Applications

Multiphase



Systems

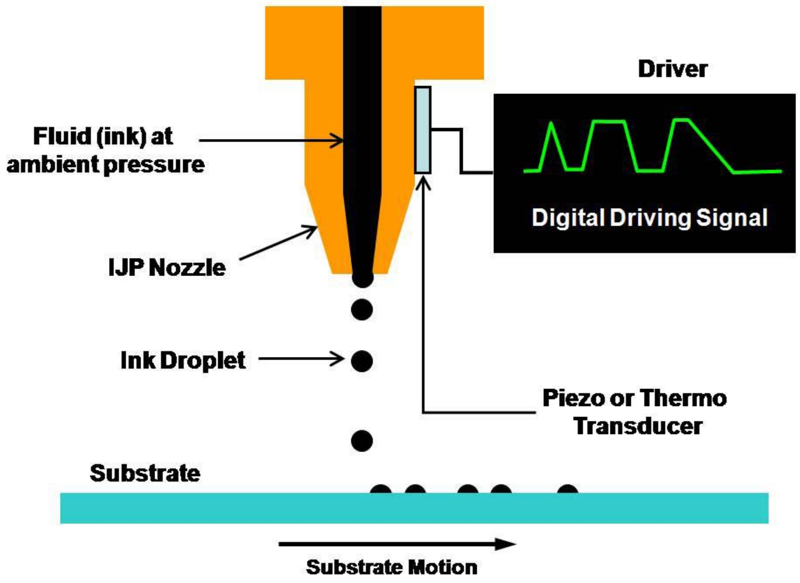
Spinodal



Decomposition

Atomization

Dynamics of drop formation from a capillary tube: inkjet printing



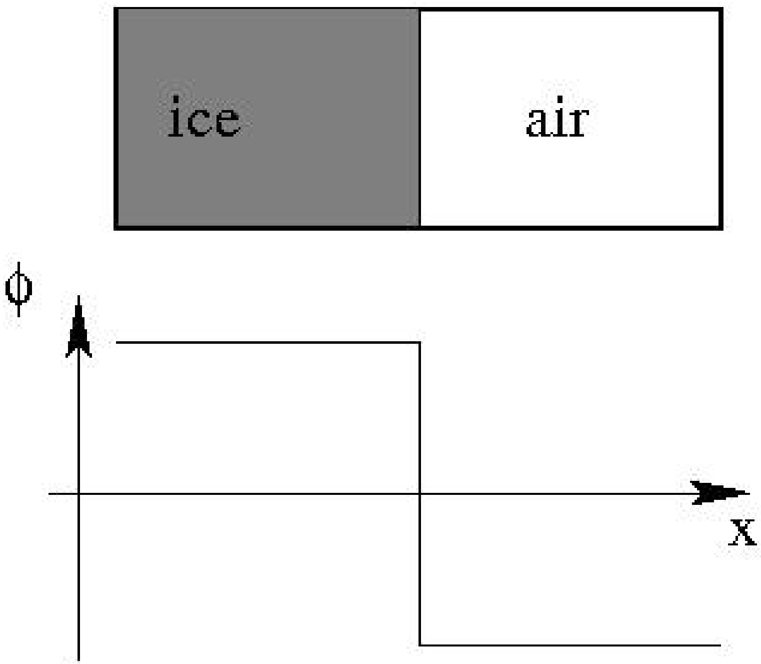
Two types of phase field models

Cahn Hillard

Phase is uniquely determined by the value of a <u>conserved field variable</u>, e.g. concentration

C < C1 we are in one phase

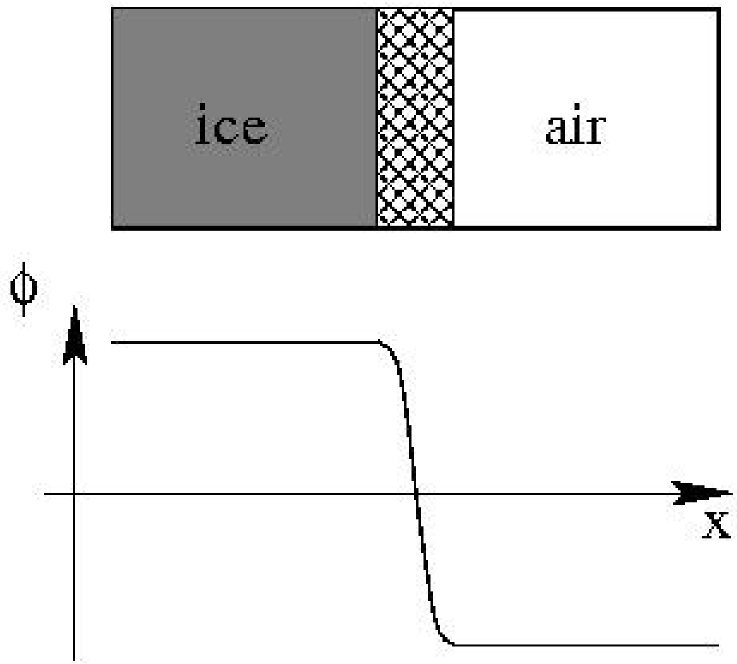
C > C2 we are in the other



Allen-Cahn

Phase is **not** uniquely determined by concentration, temperature, pressure, etc.

We define the <u>order parameter field variable</u> to determine the phase, φ



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Allen-Cahn

Free Energy

$$E = \int_{\Omega} \left(|\nabla \varphi| + F(\varphi) \right) dV$$

Cahn-Hilliard

$$E = \int_{\Omega} \left(|\nabla C| + F(C) \right) dV$$

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Free Energy

Allen-Cahn

$$E = \int_{\Omega} \left(|\nabla \varphi| + F(\varphi) \right) dV$$

Because φ is **not** conserved

$$\frac{d\varphi}{dt} = -\gamma \frac{\delta E}{\delta \varphi}$$

Double-well potential

$$F(\varphi) = \frac{\left(\varphi^2 - 1\right)^2}{4\eta^2}$$

Cahn-Hilliard

$$E = \int_{\Omega} \left(|\nabla C| + F(C) \right) dV$$

Because C is locally conserved, according to Fick‘s second law

$$\frac{dC}{dt} = -\nabla \cdot \vec{J}$$

Allen-Cahn

Free Energy

$$E = \int_{\Omega} \left(\left| \nabla \varphi \right| + F(\varphi) \right) dV$$

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Double-well potential

$$F(\varphi) = \frac{\left(\varphi^2 - 1\right)^2}{4\eta^2}$$

Denote

$$f(\varphi) := F'(\varphi)$$

Cahn-Hilliard

$$E = \int_{\Omega} \left(\left| \nabla C \right| + F(C) \right) dV$$

Because C is locally conserved, according to Fick's second law

$$\frac{dC}{dt} = -\nabla \cdot \vec{J}$$

Define potential

$$\mu = \frac{\delta E}{\delta C} = -\Delta C + F'(C)$$

Constitutive equation

$$\vec{J} = -M(C) \nabla \mu$$

$$f(C) := F'(C)$$

Allen-Cahn Equation

$$\frac{\partial C}{\partial t} + u \cdot \nabla C = \nabla \cdot \left[M(C) \nabla \left(\Delta C - f(C) \right) \right]$$

Cahn-Hilliard Equation

$$\frac{\partial \varphi}{\partial t} + u \cdot \nabla \varphi = \gamma \left(\Delta \varphi - f(\varphi) + \xi(t) \right)$$

$$\frac{d}{dt} \int_{\Omega} \varphi \, dx = 0$$

Lagrange multiplier

$$\xi(t) = \frac{1}{|\Omega|} \int_{\Omega} f(\varphi(x,t)) \, dx$$

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Momentum equation with continuity condition

$$\frac{\partial u}{\partial t} + (u \cdot \nabla) u - \nu \Delta u + \nabla p = \lambda \nabla \cdot (\nabla \varphi \otimes \nabla \varphi) + g$$

$$\nabla \cdot u = 0$$

Lagrange multiplier

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Exploitingthe expression

$$\nabla \varphi \otimes \nabla \varphi = \Delta \varphi \nabla \varphi + \frac{\nabla |\nabla \varphi|^2}{2}$$

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+IC & BC

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Allen-Cahn Problem

$$\frac{\partial u}{\partial t}+(u\cdot\nabla)u-\nu\Delta u+\nabla p_1=-\lambda_1\Delta\varphi\nabla\varphi+g_1$$

$$\frac{\partial\varphi}{\partial t}+u\cdot\nabla\varphi=\gamma_1\left(\Delta\varphi-f_1(\varphi)+\xi(t)\right)$$

$$\xi(t)=\frac{1}{|\Omega|}\int_\Omega f_1(\varphi(x,t))\,dx,\quad \frac{d}{dt}\int_\Omega\varphi(x,t)\,dx=0$$

Initial conditions

$$u(x,0)=u_0(x),\quad x\in\Omega$$

$$C(x,0)=C_0(x),\quad x\in\Omega$$

Boundary conditions

$$u=h,\quad (x,t)\in\partial\Omega_T:=\Omega\times(0,T)$$

$$\frac{\partial\varphi}{\partial n}=0,\quad (x,t)\in\partial\Omega_T$$

Cahn-Hilliard Problem

$$\frac{\partial u}{\partial t}+(u\cdot\nabla)u-\nu\Delta u+\nabla p_2=-\lambda_2\Delta C\nabla C+g_2$$

$$\frac{\partial C}{\partial t}+u\cdot\nabla C=\gamma_2\left(\Delta w-f_2(w)\right)$$

$$w=\frac{1}{\varepsilon}\mathrm{F}'(\mathrm{C})-\varepsilon\Delta C$$

Initial conditions

$$u(x,0)=u_0(x),\quad x\in\Omega$$

$$\varphi(x,0)=\varphi_0(x),\quad x\in\Omega$$

Boundary conditions

$$u=q,\quad (x,t)\in\partial\Omega_T$$

$$\frac{\partial C}{\partial n}=0,\quad (x,t)\in\partial\Omega_T$$

$$\frac{\partial w}{\partial n}=0,\quad (x,t)\in\partial\Omega_T$$

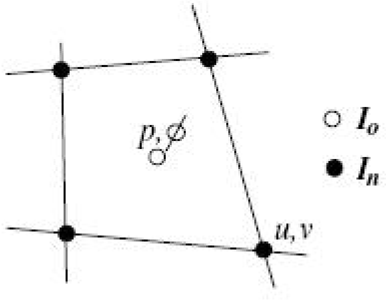
A projection method on a fixed half-staggered mesh

Step 0: Given initial data $\{\varphi^n, u^n, p^n\}$

Step1: $(\textit{the fluid evolution step})$: Compute the intermediate velocity field $\tilde{u} = (\tilde{u}, \tilde{v})$ on I_n by a semi-implicit scheme:

$$\frac{\tilde{u} - u^n}{\Delta t_n} - \nu \, \Delta_h \tilde{u} = -(u^n \cdot \nabla_h) u^n - \nabla_h p^n - \lambda \Delta_h \varphi^n \, \nabla_h \varphi^n + g(x),$$

$$\tilde{u} = 0, \quad \text{on} \quad \partial\Omega$$



Half-staggered mesh

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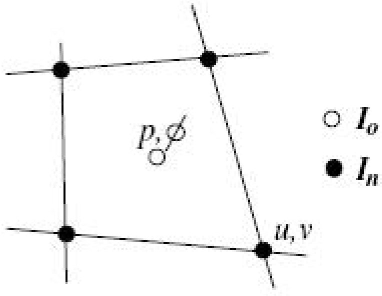

Half-staggered mesh

Step2: (the projection step) Project the intermediate velocity field onto the divergence-free vector space

$$\tilde{u} = u^{n+1} + \Delta t_n \nabla_h \psi^{n+1} \ \text{ on } \ I_n,$$

$$\nabla_h \cdot u^{n+1} = 0 \ \text{ on } \ I_0,$$

$$u^{n+1} \cdot n = 0 \ \text{ on } \ \partial\Omega,$$

Update the pressure

$$\psi^{n+1} = p^{n+1} - p^n + \nu \nabla_h \cdot \tilde{u} \ \text{ on } I_0,$$

A projection method on a fixed half-staggered mesh

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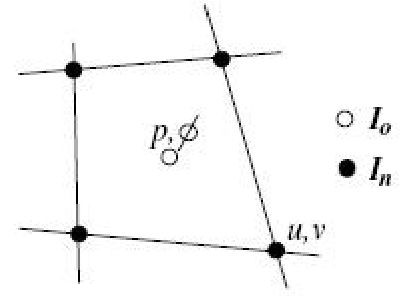

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$$\nabla_h \cdot u^{n+1} = 0 \quad \text{on} \quad I_0,$$

$$u^{n+1} \cdot n = 0 \quad \text{on} \quad \partial\Omega,$$

$\Longleftrightarrow$

Pressure-Poisson Equation

$$\Delta_h \psi = \frac{1}{\Delta t_n} \nabla_h \cdot \tilde{u}$$

$$\nabla_h \psi \cdot n = 0$$

Update the pressure

$$\psi^{n+1} = p^{n+1} - p^n + \nu \nabla_h \cdot \tilde{u} \quad \text{on} \quad I_0,$$

Step 3 (the phase evolution step): Compute the phase field by

$$\frac{\varphi^{n+1}-\varphi^{n}}{\Delta t_n}-\gamma\Delta_h\phi^{n+1}=-\nabla_h\cdot\left(u^{n+1}\varphi^{n}\right)-\gamma f\left(\varphi^{n}\right)+\gamma\xi\left(t^{n}\right)\text{ on } I_0$$

Solver for the CHNS Problem

Step 3 (the phase evolution step): Compute the phase field by

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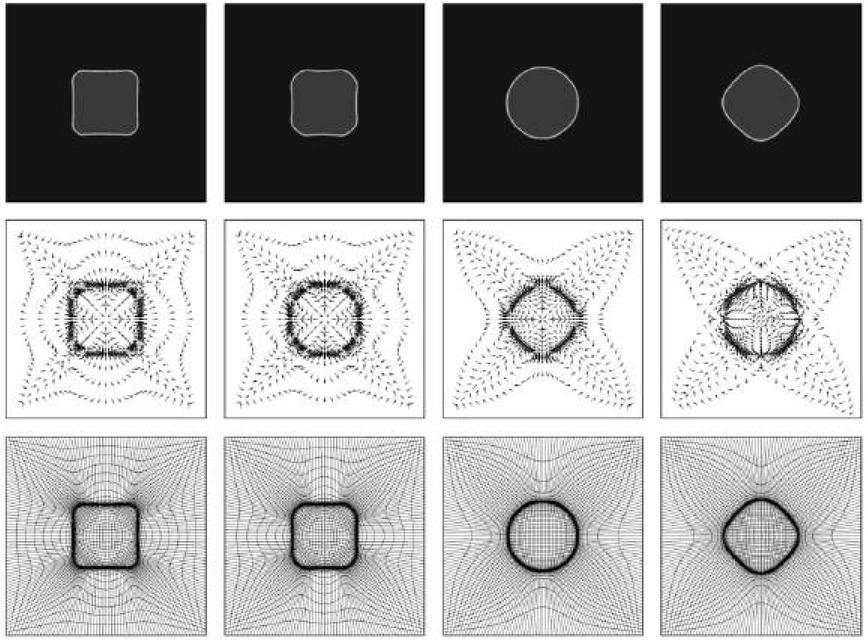
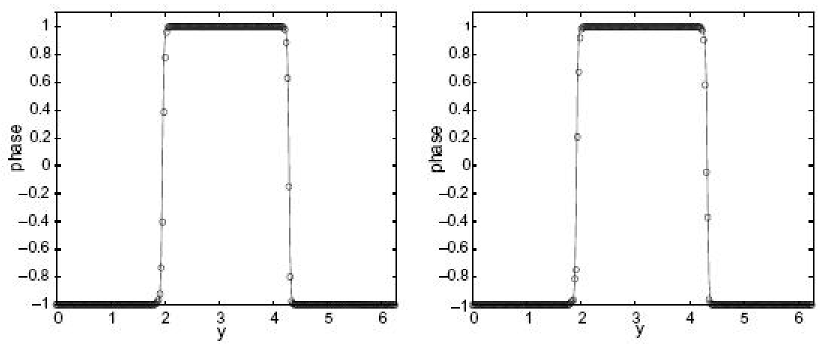
Simulation Analysis

Simulation – Surface Tension

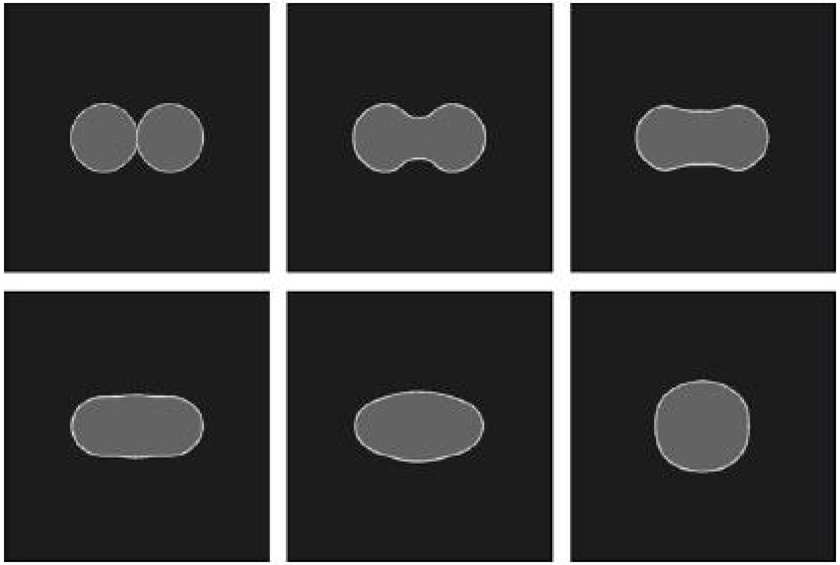


contours of the phase, the velocity fields, and mesh redistributions at $t = 0.1, 0.2, 0.3, 0.5$.

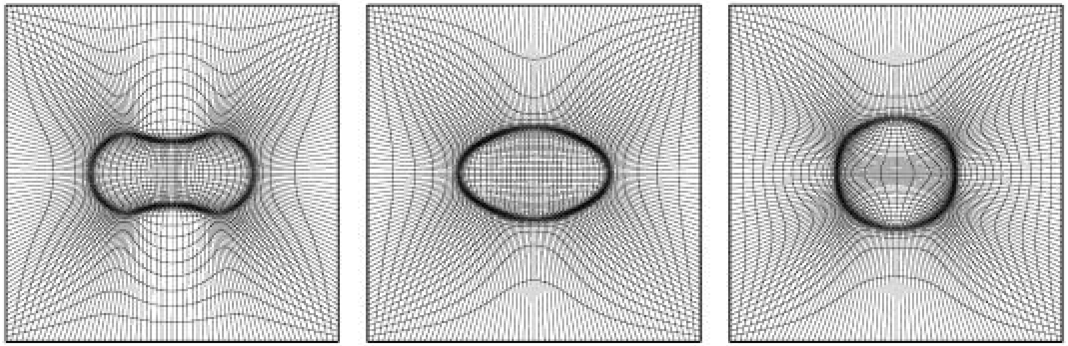


the phase ϕ along $x = \pi$. The symbol "circle" and solid line denote the adaptive solution with a resolution of 64×64 and the computed solution obtained on a 256×256 uniform mesh. Left: $t = 0.3$; right: $t = 0.5$.

Simulation – 2 Kissing Bubbles



contours of the phase ϕ at $t = 0, 0.1, 0.2, 0.3, 0.4,$ and 0.8.



the adaptive mesh distributions at $t = 0.2, 0.5,$ and 0.8.

Adaptive vs fixed mesh method

Table 1 a comparison of the CPU times (seconds) for the adaptive and fixed mesh methods

Algorithm (cell number)	$t = 0.3$	$t = 0.5$
Adaptive mesh method (64^2)	164.02	258.65
Fixed mesh method (256^2)	3716.29	5940.43

Conclusion

The phase-field method is a very versatile and robust method for studying interfacial motion in multi-component flows. It casts geometric evolution in Lagrangian coordinates into an Eulerian formulation, and provides a way to represent surface effects as bulk effects. The whole process allows us to use an energetic variational formulation that makes it possible to ensure the stability of corresponding numerical algorithms. The elastic relaxation built into the phase-field dynamics prevents the interfacial mixing layer from spreading out. Moreover, being a physically motivated approximation based on the competition between different parts of the energy functionals, the phase-field model can be adapted easily to incorporate more complex physical phenomena such as Marangoni effect and non-Newtonian rheology.

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Vielen Dank für Ihre Aufmerksamkeit!

References

Literature

- 1 Adam Powell, Introduction to Phase Field Method, Group Seminar, September 5, 2002
- 2 Xiaofeng Yang, James J. Feng, Chun Liu, Jue Shen, Numerical simulations of jet pinching-off and drop formation using an energetic variational phase-field method, Journal of Computational Physics 218 (2006) pp.417-428
- 3 Chun Liu, Jie 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
- 4 James J. Feng, Chun Liu, Jie Shen, Pengtao Yue, An energetic variational formulation with phase field methods for interfacial dynamics of complex fluids - advantages and challenges, In Modeling of soft matter, vol. 141 of IMA Vol. Math Appl., pp.1-26, Springer, New York, 2005
- 5 Yana Di, Ruo Li, Tao Tang, A General Moving Mesh Framework in 3D and its Application for Simulating the Mixture of Multi-Phase Flows, Communications in Computational Physics, Vol. 3, No.3, pp.582-602
- 6 C.M. Elliott, D.A. French, and F.A. Milner, A Second Order Splitting Method for the Cahn-Hillard Equation, Numer Math. 54, 575-590 (1989)
- 7 David Kay, Richard Welford, A Multigrid Finite Element Solver for the Cahn-Hilliard Equation, Journal of Computational Physics, Volume 212, Issue 1, (2006), pp.288-304
- 8 David Kay, Richard Welford, Efficient Numerical Solution of Cahn-Hillard-Navier-Stokes Fluids in 2D, SIAM J. Sci. Comput. Vol 29, No. 6, pp. 2241-2257
- 9 C.M. Elliott, The Cahn-Hillard model for the kinetics of phase separation, in Mathematical Models for Phase Problems, Internat, Ser. Numer. Math. 88, Birkhäuser-Verlag, Basel, Switzerland, 1989, pp. 35-73
- 10 Zhengru Zhang, Huazhong Tang, An adaptive phase field method fort he mixture of two incompressible fluids, Computers & Fluids 36, (2007), pp.1307-1318

Allen-Cahn-Navier-Stokes Problem

Momentum equation with continuity condition

$$\frac{\partial u}{\partial t} + (u\cdot\nabla)u - \nu\Delta u + \nabla p = \lambda\nabla\cdot(\nabla\varphi\otimes\nabla\varphi) + g$$

$$\nabla\cdot u = 0$$

Allen-Cahn Equation

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$$\varphi\big|_{t=0} = \varphi_0(x), \quad x\in\Omega$$

Boundary conditions

$$u = h, \quad (x,t)\in\partial\Omega_T := \Omega\times(0,T)$$

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