



Norwegian University of
Science and Technology

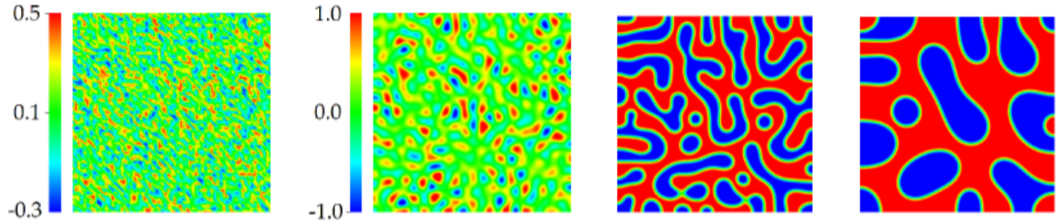
SIMULATION OF PHASE SEPARATION IN BINARY MIXTURES

Or: How to solve the Cahn-Hilliard equation with 40 lines of code

André Massing

March 21, 2025

The Cahn-Hilliard equation is ubiquitous in science and engineering



Phase separation in metall alloys during rapid quenching [Cahn and Hilliard \[1958\]](#) (Example taken from [Bosch \[2016\]](#))

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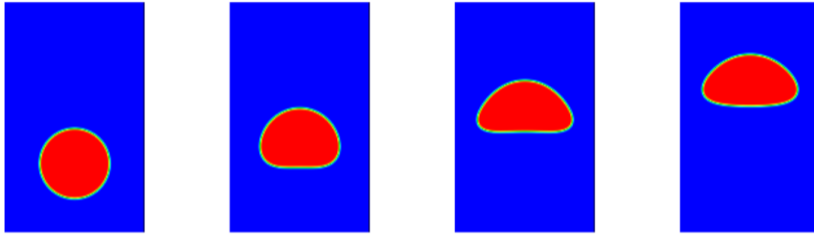
(a) Destroyed image.



(b) Reconstructed image.

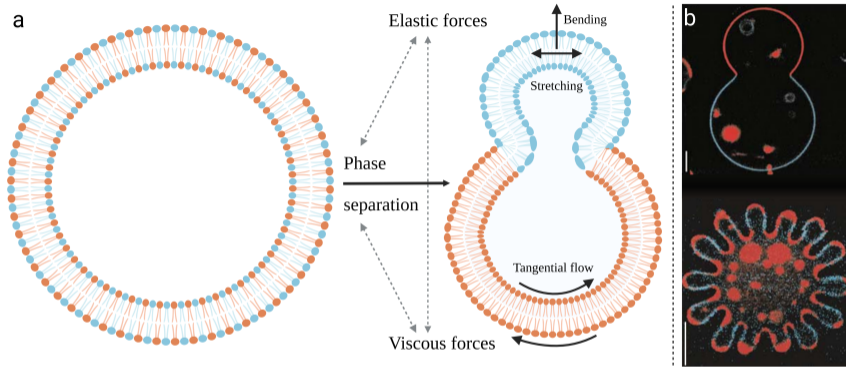
Image inpainting [Bertozzi et al. \[2007\]](#) (Example taken from [Bosch \[2016\]](#))

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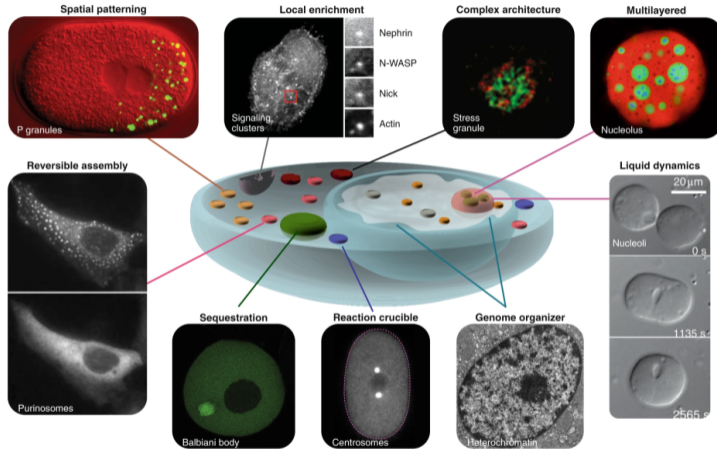
Phase-field/diffuse interface methods for moving interface [Du and Feng \[2020\]](#), e.g. for two-phase flows [Yue et al. \[2004\]](#) (Example taken from [Bosch \[2016\]](#))

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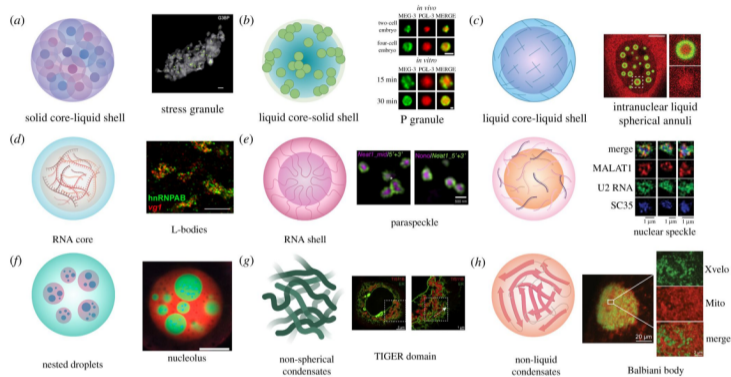
Phase separation of lipids mixture in cell membranes, Baumgart et al. [2003], Wang and Du [2008], Du et al. [2011], Elliott and Ranner [2015], Yushutin et al. [2019]

Liquid-liquid phase separation plays also a crucial role in the intracellular organization and dynamics



Bracha et al. [2019]

Liquid-liquid phase separation plays also a crucial role in the intracellular organization and dynamics



Fare et al. [2021]

Shin and Brangwynne [2017], Hyman et al. [2014], Weber et al. [2019]

The Cahn-Hilliard equation is a 4th order nonlinear parabolic problem

Mass-conservative two-component system described by (rescaled) concentration u of component 1 and $-u$ of component 2:

$$\partial_t u = \nabla \cdot (M \nabla \mu), \quad \mu = \frac{\delta \Psi_\Omega}{\delta u} = -\kappa \Delta u + f(u) \quad \text{on } \Omega \times (0, T)$$

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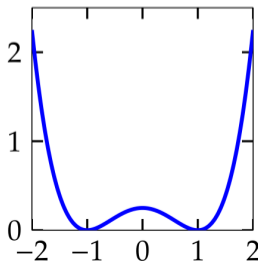
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Ginzburg-Landau free energy

$$\Psi_\Omega(u, \nabla u) = \int_\Omega \left(F(u) + \frac{\kappa}{2} |\nabla u|^2 \right) dx$$

Mobility M (constant and $= 1$)

Gradient energy coefficient $\kappa = \epsilon^2$



$$F(u) = \frac{1}{4}(u^2 - 1)^2$$

References I

- Tobias Baumgart, Samuel T Hess, and Watt W Webb. Imaging coexisting fluid domains in biomembrane models coupling curvature and line tension. *Nature*, 425(6960):821, 2003.
- Andrea L. Bertozzi, Selim Esedoglu, and Alan Gillette. Inpainting of Binary Images Using the Cahn–Hilliard Equation. *IEEE Transactions on Image Processing*, 16(1):285–291, January 2007. ISSN 1941-0042. doi: 10/fkp64c.
- J. Bosch. *Fast Iterative Solvers for Cahn–Hilliard Problems*. PhD thesis, Faculty of Mathematics, Otto-von-Guericke-Universität Magdeburg, June 2016.
- Dan Bracha, Mackenzie T. Walls, and Clifford P. Brangwynne. Probing and engineering liquid-phase organelles. *Nat Biotechnol*, 37(12):1435–1445, December 2019. ISSN 1546-1696. doi: 10/gmwx5w.
- John W Cahn and John E Hilliard. Free energy of a nonuniform system. I. Interfacial free energy. *The Journal of chemical physics*, 28(2):258–267, 1958. doi: 10/d34945.
- Qiang Du and Xiaobing Feng. Chapter 5 - The phase field method for geometric moving interfaces and their numerical approximations. In Andrea Bonito and Ricardo H. Nochetto, editors, *Handbook of Numerical Analysis*, volume 21 of *Handbook of Numerical Analysis*, pages 425–508. Elsevier, 2020.

References II

- Qiang Du, Lili Ju, and Li Tian. Finite element approximation of the Cahn–Hilliard equation on surfaces. *Comput. Methods Appl. Mech. Eng.*, 200(29-32):2458–2470, 2011. doi: 10/b6fx7k.
- Charles M Elliott and Thomas Ranner. Evolving surface finite element method for the Cahn–Hilliard equation. *Numer. Math.*, 129(3):483–534, 2015. doi: 10/f63pv8.
- Charlotte M. Fare, Alexis Villani, Lauren E. Drake, and James Shorter. Higher-order organization of biomolecular condensates. *Open Biology*, 11(6):210137, June 2021. doi: 10/gsbmp8.
- Anthony A. Hyman, Christoph A. Weber, and Frank Jülicher. Liquid-liquid phase separation in biology. *Annu. Rev. Cell Dev. Biol.*, 30(1):39–58, 2014. doi: 10/gfw8zx.
- Yongdae Shin and Clifford P. Brangwynne. Liquid phase condensation in cell physiology and disease. *Science*, 357(6357):eaaf4382, September 2017. doi: 10/gbz76s.
- Xiaoqiang Wang and Qiang Du. Modelling and simulations of multi-component lipid membranes and open membranes via diffuse interface approaches. *J. Math. Biol.*, 56(3): 347–371, 2008.
- Christoph A. Weber, David Zwicker, Frank Jülicher, and Chiu Fan Lee. Physics of active emulsions. *Rep. Prog. Phys.*, 82(6):064601, April 2019. doi: 10/ggc79h.

References III

- Pengtao Yue, James J Feng, Chun Liu, and Jie Shen. A diffuse-interface method for simulating two-phase flows of complex fluids. *J. Fluid Mech.*, 515:293–317, 2004.
- Vladimir Yushutin, Annalisa Quaini, Sheereen Majd, and Maxim Olshanskii. A computational study of lateral phase separation in biological membranes. *International journal for numerical methods in biomedical engineering*, 35(3):e3181, 2019.

