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MIXED VARIATIONAL POTENTIALS FOR CAHN-HILLARD–TYPE DIFFUSIVE PHASE SEPARATION IN SOLIDS UNDERGOING FINITE STRAINS

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Cahn-Hilliard type diffusive phase separation has ever since subsumed a large variety of processes relating to the formation of microstructures and hence demands a profound understanding of the underlying theory. This work shows that the diffusive phase separation of Cahn-Hilliard type bases upon an intrinsic *mixed variational principle*, that determines the rate of concentration and the chemical potential. The principle characterizes a new, canonically compact model structure, where the two balances involved for the species content and microforce appear as the Euler equations of the variational statement.

In addition to the modeling of pure diffusive phase separation, the Cahn-Hilliard framework can be extended to account for finite elastic deformation. To this end, the variational statement is enriched by mechanical terms accounting for an *elastic bulk response*, and the mechanical equilibrium condition is obtained as an additional Euler equation. Moreover, the gradient-enhanced Cahn-Hilliard type diffusion can be transformed to standard Fickian-type diffusion by degradation of the constitutive definition of the chemical potential, allowing an even broader application to diffusion-deformation processes.

These different types of transport phenomena in solids are embedded into the variational statement yielding an *inherent symmetry* of the underlying problem. The variational principle can be exploited in the numerical implementation by the construction of time- and space-discrete *incremental potentials*, which fully determine the update problems of typical time stepping procedures. This approach provides the most fundamental approach to the finite element solution of the Cahn-Hilliard equation based on *low order* basis functions, leading to monolithic *symmetric algebraic systems* of iterative update procedures based on a linearization of the nonlinear problem. They induce in a natural format the choice of *symmetric solvers* for Newton-type iterative updates, providing a speedup and reduction of data storage when compared with non-symmetric implementations. In this sense, the potentials developed are believed to be fundamental ingredients to a deeper understanding of the Cahn-Hilliard theory.

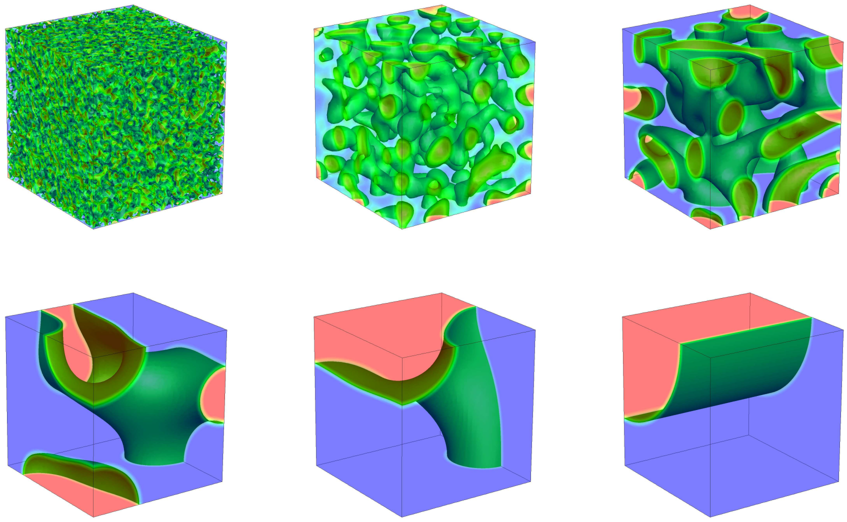

Figure 1: Diffusive phase separation in a binary mixture: Simulation of the spinodal decomposition of a homogeneously mixed binary alloy that favors two phases with small and large volume fractions.

References

[1] J.W. Cahn and J.E. Hilliard. Free energy of a nonuniform system. I. interfacial free energy. *The Journal of Chemical Physics*, 28:258–267, 1958.

[2] M.E. Gurtin. Generalized ginzburg-landau and cahn-hilliard equations based on a microforce balance. *Physica D*, 92(3-4):178–192, 1996.

[3] F.E. Hildebrand and C. Miehe. A phase field model for the formation and evolution of martensitic laminate microstructure at finite strains. *Philosophical Magazine*, 92: 4250–4290, 2012.

[4] C. Miehe. A multi-field incremental variational framework for gradient-extended standard dissipative solids. *Journal of the Mechanics and Physics of Solids*, 59:898–923, 2011.

[5] C. Miehe, F.E. Hildebrand, and L. Böger. Mixed variational potentials and inherent symmetries of the cahn–hilliard theory of diffusive phase separation. *Proceedings of the Royal Society /A*, in press, 2013.

[6] C. Miehe, S. Mauthe, and H. Ulmer. Formulation and numerical exploitation of mixed variational principles for coupled problems of cahn-hilliard-type and standard diffusion in elastic solids. *International Journal for Numerical Methods in Engineering*, submitted, 2013.

[7] L. Zhang, M.R. Tonks, D. Gaston, J.W. Peterson, D. Andrs, P.C. Millett, and B.S. Biner. A quantitative comparison between and elements for solving the cahn-hilliard equation. *Journal of Computational Physics*, 236(0):74 – 80, 2013.