High-performance phase-field modeling

P. Vignal†, A. Sarmiento†, A.M.A. Côrtes†, L. Dalcin†§, N. Collier+, V.M. Calo†⋆

†*Center for Numerical Porous Media, King Abdullah University of Science and Technology, Thuwal, Saudi Arabia, email: victor.calo@kaust.edu.sa

§Consejo Nacional de Investigaciones Científicas y Técnicas, Santa Fe, Argentina

+Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA

ABSTRACT

Many processes in engineering and sciences involve the evolution of interfaces. Among the mathematical frameworks developed to model these types of problems, the phase-field method has emerged as a possible solution. Phase-fields nonetheless lead to complex nonlinear, high-order partial differential equations, whose solution poses mathematical and computational challenges. Guaranteeing some of the physical properties of the equations has lead to the development of efficient algorithms and discretizations capable of recovering said properties by construction [2, 5].

This work builds-up on these ideas, and proposes novel discretization strategies that guarantee numerical energy dissipation for both conserved and non-conserved phase-field models. The temporal discretization is based on a novel method which relies on Taylor series and ensures strong energy stability. It is second-order accurate, and can also be rendered linear to speed-up the solution process [4]. The spatial discretization relies on Isogeometric Analysis, a finite element method that possesses the k-refinement technology and enables the generation of high-order, high-continuity basis functions. These basis functions are well suited to handle the high-order operators present in phase-field models.

Two-dimensional and three dimensional results of the Allen-Cahn, Cahn-Hilliard, Swift-Hohenberg and phase-field crystal equation will be presented, which corroborate the theoretical findings, and illustrate the robustness of the method. Results related to more challenging examples, namely the Navier-Stokes Cahn-Hilliard and a diffusion-reaction Cahn-Hilliard system, will also be presented. The implementation was done in PetIGA and PetIGA-MF, high-performance Isogeometric Analysis frameworks [1, 3], designed to handle non-linear, time-dependent problems.

REFERENCES

[1] N. Collier, L. Dalcin, and V. M. Calo. PetIGA: High-performance isogeometric analysis. *arxiv*, (1305.4452), 2013. http://arxiv.org/abs/1305.4452.

[2] H. Gómez and X. Nogueira. An unconditionally energy-stable method for the phase field crystal equation. *Computer Methods in Applied Mechanics and Engineering*, 249-252(0):52–61, 2012.

[3] A. Sarmiento, A. M. A. Cortes, D. Garcia, L. Dalcin, N. Collier, and V. M. Calo. PetIGA-MF: a multi-field high-performance implementation of divergence-conforming b-splines. *in preparation*, 2015.

[4] P. Vignal, L. Dalcin, D. L. Brown, and V. M. Calo. Linear, unconditionally energy-stable time-integrators for phase-field models. *in preparation*, 2015.

[5] X. Wu, G.J. van Zwieten, and K.G. van der Zee. Stabilized second-order convex splitting schemes for Cahn-Hilliard models with application to diffuse-interface tumor-growth models. *Int. J. Numer. Meth. Biomed. Engng.*, 2013.