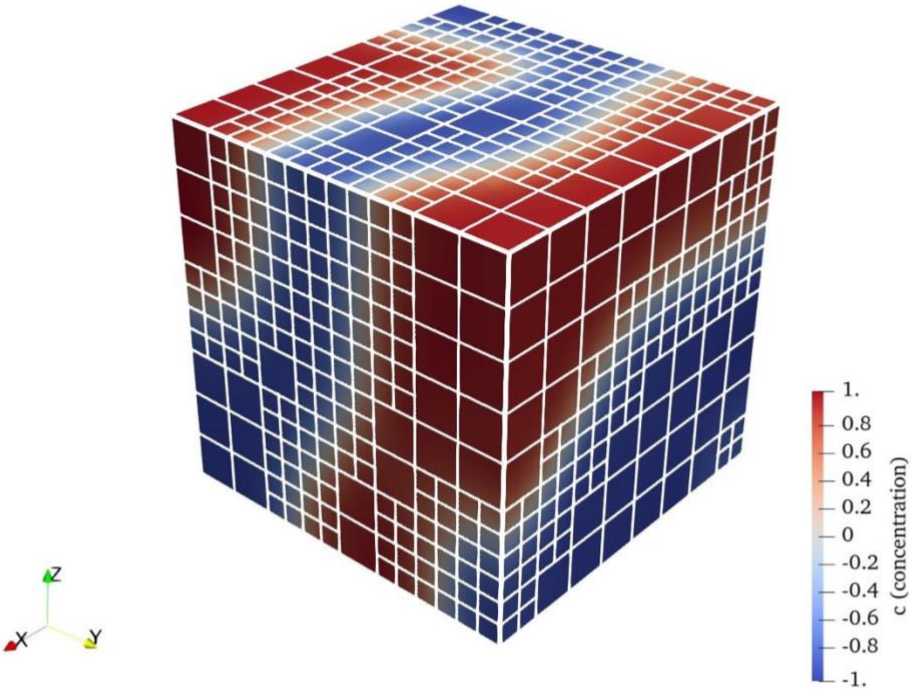
Gecko

Design for IGA-type discretization workflows

Gecko Technical Report 1

DC6 – Lucas Venta Viñuela



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Executive summary

We have explored the phase-field approach with the aim of modeling brittle and ductile fracture using Isogeometric Analysis (IGA). The focus is on high-order phase-field formulations, notably the Cahn-Hilliard equation, used to simulate phase separation phenomena. The smooth basis functions of IGA simplify the resolution of fourth-order spatial derivatives, enabling enhanced accuracy and computational efficiency compared to second-order models, even with coarser meshes. Adaptive refinement schemes using truncated hierarchical B-splines (THB-splines) further optimize computational costs by focusing resolution in regions with high gradients.

Initial results showcase the effectiveness of these methods for studying interface problems. Future work will explore adaptive immersed methods, to address challenges in complex geometry parametrization and multiphysics problems, advancing IGA's integration with CAD and expanding its application scope.

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2. List of abbreviations

CAE	*Computer-Aided Engineering*
FCM	*Finite Cell Method*
FEM	*Finite Element Method*
IGA	*IsoGeometric Analysis*

3. Introduction

This report highlights some of the outcomes of my recent research work and the potential of phase-field modeling to describe phase separation problems. This document begins with a short explanation of the importance of Isogeometric Analysis, followed by a general description of phase-field model formulations and adaptive schemes in the context of IGA. Finally, the main conclusions of this work are presented, along with an outlook on future research.

Given that one of the key missions of the GECKO network is to bridge the gap between Computer-Aided Design (CAD) and Computer-Aided Engineering (CAE), we provide a brief discussion on future work involving immersed boundary methods, such as the Finite Cell Method, which are key for representing intricate geometries within the analysis framework.

1. PHASE-FIELD MODELING VIA IGA

1.1. MOTIVATION

Reducing the pre-processing time when analyzing numerically solid structures and components is of relevance in industry, especially in automotive, aeronautical, mechanical industries, to name a few. During the past decades, the design process was conducted via Computer Aided Design (CAD) and the analysis by means of the widely known Finite Element Method (FEM). Both strategies are currently integrated in the design-to-analysis workflow, but an intense and time-consuming pre-process work must be done in order to prepare the CAD geometry to be meshed and used by the FEM code.

Bridging the gap between the CAD and FEM approaches becomes essential and can be achieved by assessing the accuracy and capabilities of the emerging isogeometric analysis (IGA) [HCB05] techniques applied to various problems. This consists in an isogeometric approach where Non-Uniform Rational B-Spline (commonly referred to as NURBS) basis functions are employed to describe both the geometry and the unknown variables of the problem, ideally circumventing in this way the costly meshing process. The fact that even the coarsest mesh retains the CAD geometry makes a direct refinement possible without going back to the initial CAD model from which the mesh has been generated, which is especially convenient when performing calculations in highly complex geometries possibly subject to large deformations; finite element analysis, instead, needs to interact with the CAD system at every refinement step, except for very simple geometries.

1.2. HIGH-ORDER PHASE FIELD FORMULATIONS

The use of highly smooth shape functions in the analysis workflow within the Isogeometric Analysis approach has eased the resolution of advanced constitutive laws and the proposition of new models that better describe the behavior of solids in two and three dimensions. Specifically, solving damage evolution problems in the context of fracture has experienced an increasing interest upon the introduction of the variational approach to brittle fracture in [FM98] for which the numerical solution relies on the regularization in [BFM00]. In general, the phase-field approach consists in incorporating a continuous field variable - the field order parameter - that results from the regularization of a sharp interface (see Figure 1). The smooth transition between the phases eases the numerical resolution of the governing equations and brings the possibility to avoid the tedious task of tracking sharp moving interfaces [AGL15].

In this regard, the IGA framework is particularly suitable for solving high-order phase-field formulations, since the smoothness of the basis functions allows for solving the equations in their primal form and improved convergence rates, as introduced in [Bo14]. Moreover, the mentioned fourth-order model gives an accuracy compared to the second-order models with a coarser mesh, as presented in the work of [Gr24]. In particular, it is shown that fourth-order models provide results comparable to second-order models with a mesh size approximately twice as coarse, translating into overall computational savings.

Our first approach to this problem was regarding the evolution of interface problems with moving interfaces with the Cahn-Hilliard equation [CH58], which is used to simulate phase separation in multi-phase systems, since it provides an alternative description of phase-transition phenomena. Additionally, this equation serves as a model high-order phase field equation, and its implementation in this context constitutes a laying stone for understanding other complex phase-field formulations.

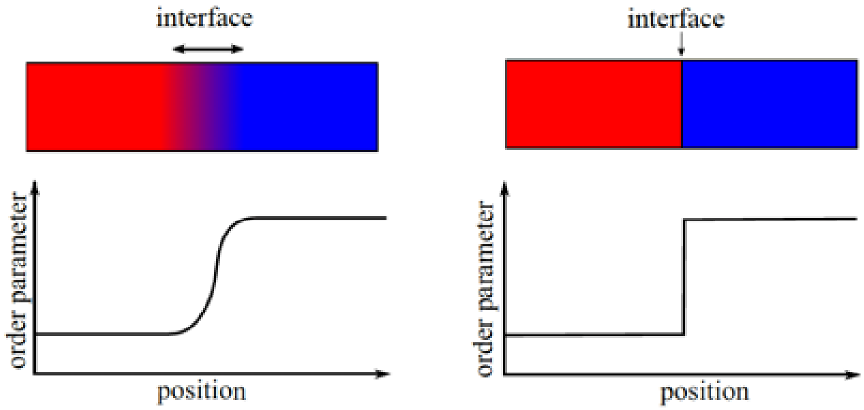

Figure 1. Schematic of phase-field and sharp-interface models [Zh17]

Specifically, the Cahn-Hilliard equation involves fourth-order spatial derivatives, where the primal variational formulation of the fourth-order operators are well-defined and integrable if the finite element basis functions are piecewise smooth and globally C^1-continuous. This requirement can be easily met within the IGA framework, since the regularity of the basis functions can be tailored. Our first goal was to develop an IGA-based phase-field implementation of the Cahn-Hilliard equation within the G+Smo framework [Gi24], an open-source *C*++ library that brings together mathematical tools for geometric design and numerical simulation. This implementation provides the foundation for introducing other higher-order phase-field models in the library and serves as a prototype for solving the Cahn-Hilliard equation on any single-patch geometry parameterization that exists therein. Figure 2 shows the evolution of the species concentration following a spinodal decomposition mechanism.

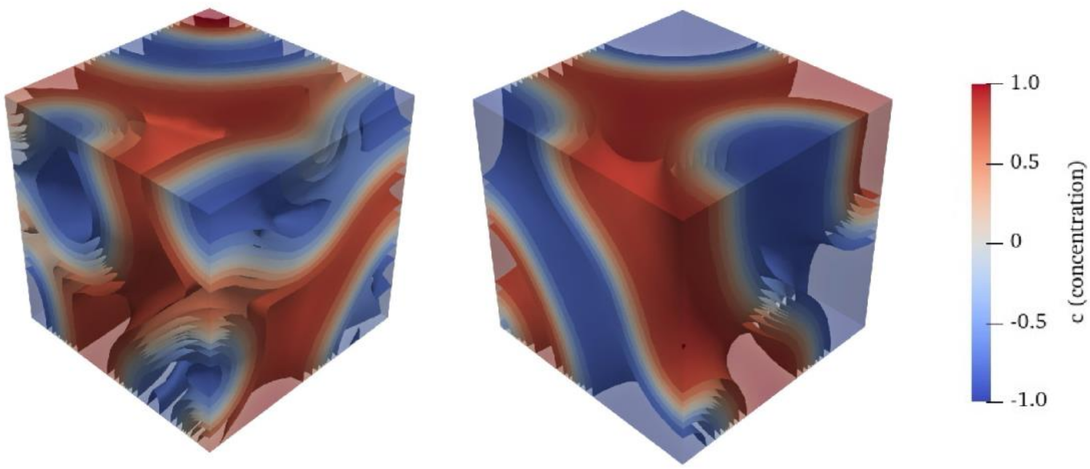

Figure 2. Evolution of the concentration from a randomly perturbed initial condition in two different time steps

1.3. ADAPTIVE IGA

In phase-field models, the width of the smooth transition between the phases is controlled by a length-scale parameter. Reducing the value of this parameter leads to convergence of a phase-field interface to a sharp interface topology, but induces locally high gradients that require high spatial resolution of the meshes [Na19] Although a uniform global h-refinement until the length-scale parameter is well resolved would be the most trivial option, this introduces excessive computational cost. Thus, it is desirable to use adaptive approaches that allow for locally refining/coarsening the mesh based on the evolution of the phase-field in the simulation [Br23].

Recently, we implemented an adaptive scheme for solving the Cahn-Hilliard equation using truncated hierarchical B-spline (THB-spline) basis functions [GJS12], which are particularly well-suited for adaptive refinement in the context of IGA, as they preserve the properties of hierarchical B-splines [Kr97] [Vu11], such as linear independence and non-negativity, and also form a partition of unity. Figure 3 illustrates our initial results with mesh adaptivity as the phase separation mechanism progresses.

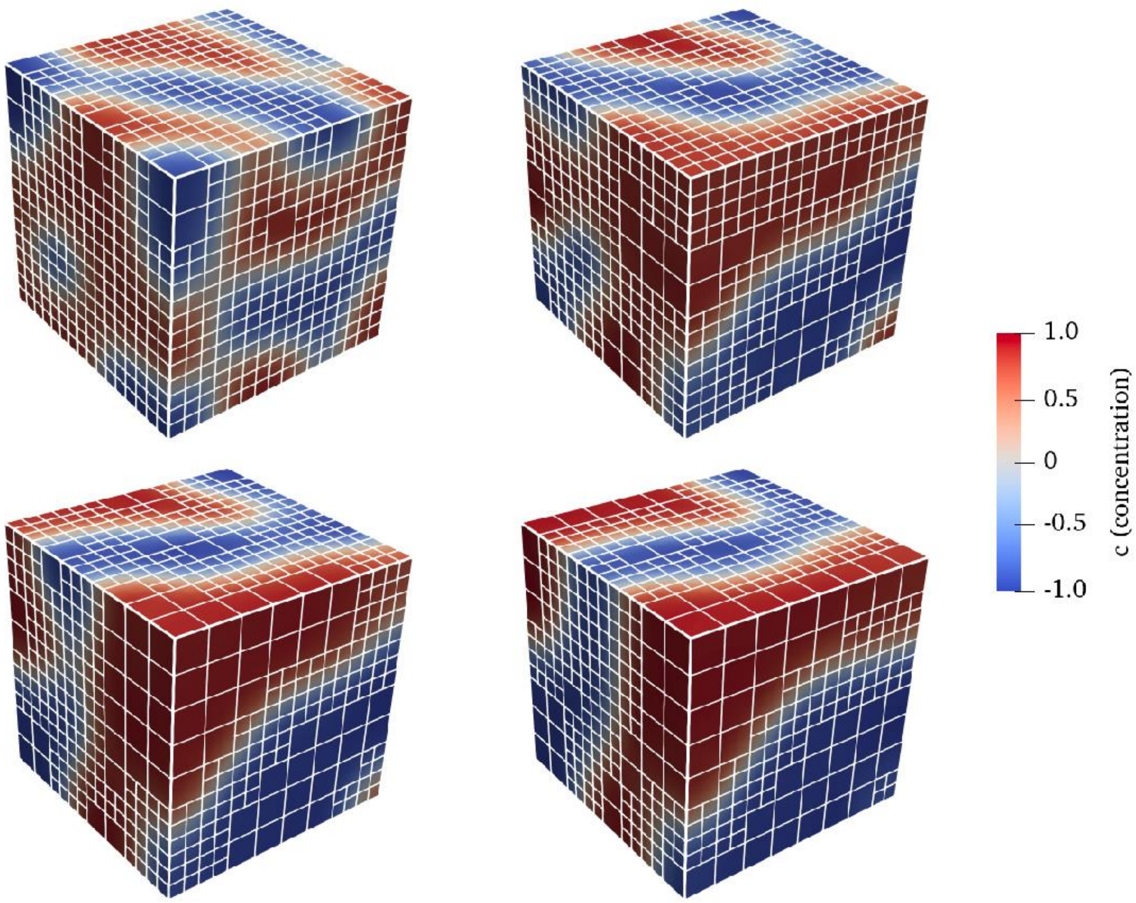

Figure 3. Evolution of the concentration from a randomly perturbed initial condition in two different time steps with mesh adaptivity. Snapshots are shown in order of increasing time step, progressing from left to right and top to bottom

2. CONCLUSIONS AND OUTLOOK

Although IGA has introduced remarkable advantages in numerical computations, it has also opened many unexpected areas of research that need to be further explored to allow for the simulation of different complex problems and its integration with CAD. To this aim, the future work on phase-field modelling will involve the development of adaptive models within the context of immersed methods. Specifically, the approach known as the Finite Cell Method (FCM) [PDR07] [Du08] allows for reproducing very complex geometries in the analysis. The study of immersed methods within the IGA framework will provide the flexibility characteristic of such methods in situations where the geometry is difficult to parametrize and will allow the study of several multiphysics problems of interest. Furthermore, an important effort in this work must be put on mesh adaptivity and sensitivity, as well as locally refinable spline constructions in the context of higher-order phase-field models, to investigate both phase separation phenomena and brittle and ductile fracture.

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