

ENERGY-STABLE TIME DISCRETIZATIONS FOR THE PHASE-FIELD CRYSTAL EQUATION

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Modeling of phase-transitions has garnered a lot of interest in recent years, and the solution to these problems through the use of phase-field methods looks very promising. Unfortunately, the phase-field framework as a method, leads to nonlinear and high-order partial differential equations [1]. These equations, not easily solved using standard numerical methods, have lead to interesting numerical algorithms to handle them, that look to ensure different problem-related properties such as conservation of mass and energy-stability. Among the methods that have been tried out in finite element settings, Isogeometric Analysis (IGA) [2] has stood out for the ease with which the higher-order, globally continuous basis functions can be generated.

In this work, we analyze different possible discretizations using IGA to solve the phase-field crystal equation, a nonlinear, time-dependent, sixth-order partial differential equation. Using arguments from [3], we are able to prove energy-stability and second-order accuracy in time. Comparisons are done against the state of the art [4], and their behaviour in terms of convergence in a free-energy sense is analyzed. Implementation was done using PetIGA, a high performance Isogeometric Analysis framework. It is heavily based on PETSc, and designed to handle non-linear, time-dependent problems [5]. Two-dimensional and three-dimensional examples are presented, involving crystalline growth.

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