Isogeometric analysis and unconditional time integration of the phase field crystal equation

The phase-field crystal equation has been recently put forward as a model for microstructure evolution of two-phase systems on atomic length and diffusive time scales. The theory is cast in terms of an evolutive nonlinear sixth-order partial differential equation for the interatomic density that locally minimizes an energy functional with the constraint of mass conservation. I will present a new numerical algorithm for the phase-field crystal equation that is second-order time-accurate and unconditionally stable with respect to the energy functional. I will show several numerical examples in two and three dimensions dealing with crystal growth in a supercooled liquid and crack propagation in a ductile material. These examples show the effectiveness of our new algorithm.

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