

数学与系统科学研究院
计算数学所定期学术报告

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报告题目:

An energy stable pseudo-spectral
numerical scheme for the square
phase field crystal (SPFC) equation

邀请人: 谢和虎 研究员

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报告地点: 数学院南楼二层

204 教室

Abstract:

An energy stable numerical scheme is proposed and analyzed for the square phase field crystal (SPFC) equation, a gradient flow to model the crystal dynamics at the atomic scale in space but on diffusive scales in time. In particular, a modification of the free energy potential to the standard phase field crystal model leads to a composition of the 4-Laplacian and the regular Laplacian operators. The Fourier pseudo-spectral approximation is taken in space, so that the summation in parts formulas enable one to study the discrete energy stability for such a high order spatial discretization. In the temporal approximation, a second order BDF stencil is applied in the time direction, combined with an appropriate extrapolation for the concave diffusion term. At a theoretical level, the unique solvability, energy stability are established, and an optimal rate convergence analysis is derived. In the numerical implementation, the preconditioned steepest descent (PSD) iteration is applied to solve for the composition of the highly nonlinear 4-Laplacian term and the standard Laplacian term, and a geometric convergence is assured for such an iteration. A few numerical experiments are also presented.

欢迎大家参加！