



复旦大学数学科学学院 数学综合报告会

报告题目: A second order scalar auxiliary variable (SAV) numerical method for the square phase field crystal (SPFC) equation and its comparison with direct nonlinear solver

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时间: 2020-6-23 星期二 11:00-12:00

地点: Zoom meeting ID: 632 8423 6328, Password: 200623

报告摘要:

A second order accurate (in time), scalar auxiliary variable (SAV)-based 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. 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 combined with the SAV approach. In particular, an appropriate decomposition for the physical energy functional is formulated, so that the nonlinear energy part has a well-established global lower bound, and the rest terms lead to constant-coefficient diffusion terms with positive eigenvalues. In turn, the numerical scheme could be very efficiently implemented by constant-coefficient Poisson-like type solvers (via FFT), and energy stability is established by introducing an auxiliary variable, and an optimal rate convergence analysis is provided for the proposed SAV method. A few numerical experiments are presented, and a careful numerical comparison with direct nonlinear solvers is also undertaken.

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