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Gradient-Stable Linear Time Steps for Phase Field Models BENJAMIN VOLLMAYR-LEE, Bucknell University — Phase field models, which are nonlinear partial-differential equations, are a widely used for modeling the dynamics and equilibrium properties of materials. Unfortunately, time marching the equations of motion by explicit methods is usually numerically unstable unless the size of the time step is kept below a lattice-dependent threshold. Consequently, the amount of numerical computation is determined by avoidance of the instability rather than by the natural time scale of the dynamics. This can be a severe overhead. In contrast, a gradient stable method ensures a decreasing free energy, consistent with the relaxational dynamics of the continuous time model. Eyre's theorem proved that gradient stable schemes are possible, and Eyre presented a framework for constructing gradient-stable, semi-implicit time steps for a given phase-field model. Here I present a new theorem that provides a broader class of gradient-stable steps, in particular ones in which the implicit part of the equation is linear. This enables use of fast Fourier transforms to solve for the updated field, providing a considerable advantage in speed and simplicity. Examples will be presented for the Allen-Cahn and Cahn-Hilliard equations, an Ehrlich-Schwoebel-type interface growth model, and block copolymers.

Benjamin Vollmayr-Lee
Bucknell University

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