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New linear schemes for a Cahn Hilliard diffuse interface model

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Resumen

The study of interfacial dynamics in the mixture of different fluids, solids, or gas is one of the fundamental issues in hydrodynamics and materials science due it plays an increasingly important role in many current scientific, engineering, and industrial applications. Traditional fluid dynamics treats these mixtures as sharp interfaces on which a set of interfacial balance conditions must be imposed. It is delicate and difficult to develop a proper notion of generalized solutions of these models and it becomes even more challenging to compute the generalized solutions when they are defined, leading to an almost intractable theoretical problem. An alternative approach for solving interface problems is the diffuse interface theory, which describes the interface by a mixing energy represented as a layer of small thickness. The method uses an auxiliary function (so-called phase-field function) to localize the phases, assuming distinct values in the bulk phases (for instance 1 in a phase and -1 in the other one) away from the interfacial regions over which the phase function varies smoothly. The Cahn-Hilliard model describes the complicated phase separation and coarsening phenomena in the mixture of different fluids, solid or gas where only two different concentration phases can exist stably. The Cahn-Hilliard equation (supplemented with initial and boundary conditions)

$$\phi_t - \Delta(-\Delta\phi + f(\phi)) = 0$$

is a gradient flow of the total free energy functional,

$$E(\phi) = \int_\Omega \left(\frac{1}{2}|\nabla\phi|^2 + F(\phi) \right) dx$$

where ϕ represents the phase field function and $F(\phi)$ is a double well potential, with $F'(\phi) = f(\phi)$. This work is devoted to comparing different linear schemes to approximate the model when we consider the polynomial potential $F(\phi) = \frac{1}{4\varepsilon^2}(\phi^2 - 1)^2$. We have developed two new linear schemes, where the first one is based on introducing a Lagrange multiplier in order to obtain a unconditionally stable linear scheme. This idea has been previously introduced to deal with nematic liquid crystal flows. Meanwhile, in the second one we have developed a second-order in time approximation of the potential term following the ideas introduced in previous works. We also present the results of some numerical simulations that we have carried out using these two new schemes and other commonly used linear schemes.

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