UNIFORM L^p-BOUND OF THE ALLEN–CAHN EQUATION AND ITS NUMERICAL DISCRETIZATION

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Abstract. We study uniform bounds associated with the Allen–Cahn equation and its numerical discretization schemes. These uniform bounds are different from, and weaker than, the conventional energy dissipation and the maximum principle, but they can be helpful in the analysis of numerical methods. In particular, we show that finite difference spatial discretization, like the original continuum model, shares the uniform L^p -bound for all even p, which also leads to the maximum principle. In comparison, a couple of other spatial discretization schemes, namely the Fourier spectral Galerkin method and spectral collocation method preserve the L^p -bound only for p = 2. Moreover, fully discretized schemes based on the Fourier collocation method for spatial discretization and Strang splitting method for time discretization also preserve the uniform L^2 -bound unconditionally.

Key words. Allen–Cahn Equations, maximum principle, operator splitting, uniform L^p -bound, Fourier spectral methods.

1. Introduction

We consider the standard Allen–Cahn (AC) equation in this paper, which is given as follows

(1)
$$\frac{\partial u}{\partial t} = \epsilon^2 \Delta u - f(u), \quad \mathbf{x} \in \Omega, t \in (0, T],$$
$$u(\mathbf{x}, 0) = u_0(\mathbf{x}), \quad \mathbf{x} \in \bar{\Omega},$$

where u = u(x,t) is a real-valued scalar function, the nonlinear term is given by $f(u) = u^3 - u$, the parameter $\epsilon > 0$ characterizes the width of diffuse interface, and Ω is a bounded domain in \mathbb{R}^d . We restrict our attention to the periodic boundary condition with Ω being the unit cell. The Allen–Cahn equation can be viewed as an L^2 -gradient flow of the following Ginzburg-Landau free energy functional

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

where F(u) is taken as the typical double well potential $F(u) = \frac{1}{4}(u^2 - 1)^2$ so that f(u) = F'(u). We also assume that the initial data $u_0 = u_0(x)$ takes value between the energy wells, i.e., bounded by the constant 1.

The Allen–Cahn equation has been introduced by Allen and Cahn in [1] to describe the motion of anti-phase boundaries in crystalline solids. The equation also bears other names, for example, the Ginzburg-Landau equation where the unknown solution may be real, complex, or vector-valued [8, 21]. It is now a basic model equation for the diffuse interface (phase field) approach developed to study phase transitions and interfacial dynamics in materials science as well as various problems in many other applications [4, 7]. There have also been extensive numerical studies of phase field and diffuse interface models, see, e.g. [6, 16, 20].

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One of the important issues concerning numerical solution of differential equations is the stability of numerical schemes. For nonlinear models, a priori bounds on the discrete solutions are often important to the numerical stability. Given AC being a typical gradient flow, we have

$$\frac{d}{dt}E = -\|u_t\|_2^2 \le 0 \text{ and } E(t) \le E(0),$$

which represents the energy bound of the original continuum model. The preservation of such nonlinear energy bounds by numerical approximations often dominates the discussions in numerical analysis, In [11], Eyre proposed an unconditionally stable energy convex splitting scheme for general gradient flows, but it is only first order. Some recent stability analysis can be found in [12, 13, 14, 24, 28, 29], where most authors again focused on the energy dissipation.

Another intrinsic bound for the Allen–Cahn equation is the point-wise bound in the form of a maximum principle, see, e.g., [10]. Specifically, if the initial data $u_0(x)$ takes value between the energy wells, i.e., bounded by the constant 1, then the timedependent solution of the Allen–Cahn equation is also bounded by constant 1. Such a property can be preserved numerically on the discrete level, see for example [5, 27] for discussions on fully discrete finite volume and finite difference approximations. The discrete maximum principle was further extended to generalized Allen–Cahn equations and fractional Allen–Cahn equations [18, 23]. In these works, the space Laplace operator is discretized by central finite difference. Similar results have been established for finite volume schemes as well as finite element methods with mass lumping based on Voronoi-Delaunay meshes, see [6] and the references cited therein. However, it is known that the maximum principle can not be preserved in general by spectral methods, since the spectral projection itself may fail to retain point-wise bounds. Hence, we do not expect that spectral methods preserve the maximum principle for nonlinear Allen–Cahn equations.

In this paper, we present some bounds on solutions other than the energy bound and maximum principle for the Allen–Cahn equation and its numerical discretization. Specifically, we consider weaker L^p -bounds. First, we define the L^p -average norm $\|\|\cdot\|\|_p$ of u in the fixed domain Ω for any p > 0,

(3)
$$|||u|||_{p} = \frac{1}{S_{\Omega}} ||u||_{L^{p}(\Omega)}^{p} = \frac{1}{S_{\Omega}} \int_{\Omega} |u|^{p} dx,$$

where S_{Ω} is the volume of the domain Ω . Given the assumed bounds on the initial data, by applying the maximum principle directly, we can obtain

(4)
$$|||u|||_p(t) = \frac{1}{S_\Omega} \int_\Omega |u(x,t)|^p dx \le \frac{1}{S_\Omega} \int_\Omega 1 dx = 1,$$

which is uniform not only in space and time, but also with respect to the domain Ω , the diffuse interface width ϵ and the exponent p. This uniform L^p -bound is, of course, weaker than the maximum principle. On the other hand, the uniform L^p -bound implies the maximum principle if it holds for a sequence of p that goes to infinity. The larger p one can pick, the closer L^p -bound is to the maximum principle.

Computationally, we are often interested in constructing discrete numerical schemes that preserve the properties of the continuum equations as much as possible. However, this is not always possible for complex systems. Hence, it is interesting to know to what extent, weaker results can be established which may still allow the numerical schemes to provide reliable computational predictions. For example, it is obvious that there could be more flexibility designing numerical schemes to preserve