Average vector field method with discontinuous Galerkin finite element space discretization for Allen–Cahn equation

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Abstract. In this work, Allen–Cahn equation is discretized using symmetric interior penalty discontinuous Galerkin finite elements. Time discretization is performed by the energy stable average vector field method. The numerical results for one and two dimensional Allen-Cahn equation with periodic, Neumann and Dirichlet boundary conditions show that the numerical energy decreases monotonically, the phase separation and metastability phenomena can be observed and the ripening time is detected correctly.

Keywords. Allen–Cahn equation, gradient systems, discontinuous Galerkin method, average vector field method, time adaptivity

Preprint No. 2014-5
August 2014

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1 Introduction

Gradient flows are evolutionary systems driven by an energy, in the sense that the energy decreases along solutions as fast as possible. A typical example for gradient flow equation is the Allen–Cahn equation, modeling the reaction kinetics in reaction diffusion systems in material science. It was first introduced by Allen and Cahn [1] to describe the motion of anti-phase boundaries in crystalline solids. In the last thirty years, it has been widely used in many complicated moving interface problems in material science and fluid dynamics. The Allen-Cahn equation

\[ u_t = \varepsilon^2 \Delta u - f(u), \quad (x,t) \in \Omega \times (0,T) \]  

is investigated with suitable initial and boundary conditions in the literature intensively, where \( u \) represents the phase state between materials. The parameter \( \varepsilon \) is known as the interaction length, capturing the dominating effect of the reaction kinetics and represents the effective diffusivity. The bistable nonlinear term is \( f(u) = (u^2 - 1)u = \mathcal{F}'(u) \) with the Ginzburg–Landau double well potential

\[ \mathcal{F}(u) = \frac{(1-u^2)^2}{4} \]

Allen-Cahn equation describes the gradient flow of the Liapunov energy functional

\[ \mathcal{E}(u) = \int_{\Omega} \left( \frac{\varepsilon^2}{2} |\nabla u|^2 + \mathcal{F}(u) \right) dx \]  

minimizing \( \mathcal{E}(u) \). The energy decreasing property of the Allen-Cahn equation is obtained by taking the \( L^2 \) inner product of Eq. (1) with \( (-\varepsilon^2 \Delta u + f(u)) \)

\[ \mathcal{E}(u(t_n)) < \mathcal{E}(u(t_m)), \quad \forall t_n > t_m. \]  

Besides energy decrease, the main characteristics of the Allen-Cahn equation are phase separation, metastability and no mass conservation. In recent years, a lot of work have been devoted to developing numerical schemes for the solution of Allen-Cahn equation. For space discretization finite differences, finite elements and spectral methods are used. Most of the work is devoted to analysis and numerical studies for periodic boundary conditions. Other boundary conditions like the Neumann and Dirichlet, are considered less in the literature.

For time integration it is important to preserve the energy decreasing property (3). In the past, many energy stable integrators are developed to satisfy the energy decreasing property of the Allen-Cahn equation. For small values of the diffusion parameter \( \varepsilon \), semi-discretization leads to stiff systems. Because the explicit methods are not suitable for stiff systems and the fully implicit systems require solution of nonlinear equations at each time step, implicit-explicit (IMEX) methods are developed (see for example [19]). In the semi-implicit schemes, the linear stiff part is treated implicitly and the nonlinear part explicitly, so that for each time step a

In this work we use discontinuous Galerkin finite elements (DGFEM) for the space discretization [2, 17]. In contrast to the continuous finite elements, the DGFEMs uses the set of piecewise polynomials that are fully discontinuous at the interfaces. In this way, the DGFEM approximation allows to capture the sharp gradients or singularities that affect the numerical solution locally. Moreover, the boundary conditions are imposed weakly. Due to the local structure of the elements, DGFEMs are parallelizable. In Section 2, we will give uniform description of DGFEM semi-discretization for the Allen-Cahn equation for Dirichlet, Neumann and periodic boundary conditions. It is important to design efficient and accurate numerical schemes that are energy stable and robust with small $\epsilon$. Among the energy decreasing methods the best known is the implicit Euler method. It is strongly energy decreasing, i.e. the discrete energy decreases without any restriction for the step size $\Delta t$ for very stiff gradient systems with $\epsilon \to 0$ [13]. Higher order energy decreasing methods with orders $\geq 3$ are the discontinuous Galerkin-Petrov in time methods (with different trial and test functions) [18] and Gauss Radau IIA Runge-Kutta collocation methods [14]. But they require coupled systems of equations at each time step increasing the computational cost. The only second order implicit energy stable method is the average vector field (AVF) method [3, 13], which belongs to the calls of discrete gradient methods [16]. AVF method is a structure preserving integrator, i.e., it preserves the energy for Hamiltonian and Poisson systems [13, 6], preserves energy decreasing property for the gradient systems and for systems with Lyapunov functions. The time discretization of the DGFEM semi-discretized Allen-Cahn equation with the AVF method is developed in Section 3. The equivalence of the AVF method to the second order discontinuous Galerkin-Petrov method is also shown.

The reminder of the paper is organized as follows. In Section 2, we give the DGFEM semi-discretization of the Allen-Cahn equation. Section 3 is devoted to the time discretization with the AVF method, where solution of the nonlinear equations are described in detail. We present in Section 4 several numerical examples to demonstrate the applicability of the DGFEM discretization coupled with AVF method for the Allen-Cahn equation, where the time-adaptive algorithm for the computation of the ripening time is given. The paper ends with some conclusions.

2 Discontinuous Galerkin (DG) Space Discretization

In this section, we briefly describe the DG discretization of the Allen–Cahn equation (1). The classical weak formulation (semi–discrete) of the Allen–Cahn equa-
tion (1) reads: find \( u(t) \in H_0^1(\Omega) \) such that

\[
(u,v)_\Omega + a(u,v) + (f(u),v)_\Omega = 0, \quad \forall v \in H_0^1(\Omega), t \in (0,T]
\]

(4)

where \((\cdot,\cdot)_\Omega\) denotes the usual \( L^2 \)-inner product over the domain \( \Omega \) and \( a(u,v) = \varepsilon^2(\nabla u, \nabla v)_\Omega \) is the bilinear form. In continuous finite elements, the time-dependent approximation to the system (4) belongs to a finite dimensional conforming subspace \( V_h \subseteq H_0^1(\Omega) \). In contrast to the continuous finite elements, DG methods are suitable to use non-conforming spaces, i.e. \( V_h \not\subseteq H_0^1(\Omega) \), and to impose the Dirichlet boundary conditions weakly.

The DG discretization given in this article is based on the symmetric interior penalty Galerkin (SIPG) method, applied to the diffusion part of the problem for Dirichlet, Neumann [17], and periodic boundary conditions [21]. Let \( \mathcal{T}_h \) be a family of shape regular meshes such that \( \bar{\Omega} = \cup_{K \in \mathcal{T}_h} \bar{K} \), \( K_i \cap K_j = \emptyset \) for \( K_i, K_j \in \mathcal{T}_h \), \( i \neq j \). The diameter of an element \( K \) and the length of an edge \( E \) are denoted by \( h_K \) and \( h_E \), respectively. Set the test and trial space

\[
V_h = \{ u \in L^2(\Omega) : u|_K \in \mathbb{P}^q(K) \quad \forall K \in \mathcal{T}_h \}
\]

(5)

where \( \mathbb{P}^q(K) \) denotes the set of all polynomials on \( K \in \mathcal{T}_h \) of degree at most \( q \). We note that the trial space and the space of test functions are chosen to be the same since the boundary conditions (Dirichlet) in DG methods are imposed weakly.

We split the set of all edges \( E_h \) into the set \( E_h^0 \) of interior edges, the set \( E_h^\partial \) of Dirichlet boundary edges and the set \( E_h^N \) of Neumann boundary edges so that \( E_h = E_h^0 \cup E_h^\partial \) with \( E_h^D = E_h^\partial \cup E_h^N \). Let the edge \( E \) be a common edge for two elements \( K \) and \( K' \). For a piecewise continuous scalar function \( u \), there are two traces of \( u \) along \( E \), denoted by \( u|_E \) from inside \( K \) and \( u'|_E \) from inside \( K' \). Then, the jump and average of \( u \) across the edge \( E \) are defined as:

\[
[u] = u|_E n_K + u'|_E n_{K'}, \quad \{ u \} = \frac{1}{2} (u|_E + u'|_E).
\]

where \( n_K \) and \( n_{K'} \) denote the outward unit normal vector to the boundary of the elements \( K \) and \( K' \) on the edge \( E \), respectively. Similarly, for a piecewise continuous vector field \( \nabla u \), the jump and average across an edge \( E \) are given by

\[
|\nabla u| = \nabla u|_E \cdot n_K + \nabla u'|_E \cdot n_{K'}, \quad \{ \nabla u \} = \frac{1}{2} (\nabla u|_E + \nabla u'|_E).
\]

For a boundary edge \( E \subset K \cap \partial \Omega \), we set \( \{ \nabla u \} = \nabla u \) and \( [u] = u n \) where \( n \) is the outward unit normal vector to \( \partial \Omega \). Then, SIPG discretized, in space, problem for the Allen-Cahn equation reads: set \( u_h(0) \in V_h \) be the projection (orthogonal \( L^2 \)-projection) of the initial condition \( u_0 \) onto \( V_h \), find \( u_h(t) \in V_h \) such that

\[
(\partial_t u_h, v_h)_\Omega + a_h(u_h, v_h) + (f(u_h), v_h)_\Omega = I_h(v_h), \quad \forall v_h \in V_h, t \in (0,T],
\]

(6)
where the bilinear form is of the form \( a_h(u, v) = \tilde{a}_h(u, v) + J^2_h(u, v) \) with
\[
\tilde{a}_h(u_h, v_h) = \sum_{K \in \mathcal{T}_h} \int_K \varepsilon^2 \nabla u \cdot \nabla v - \sum_{E \in \mathcal{E}_0^h} \int_E \{\varepsilon^2 \nabla u\} \cdot [v] ds - \sum_{E \in \mathcal{E}_1^h} \int_E \{\varepsilon^2 \nabla v\} \cdot [u] ds,
\]

where the parameter \( \sigma \) is called the penalty parameter and it should be sufficiently large to ensure the stability of the DG discretization as described in [17] with a lower bound depending only on the polynomial degree. The bilinear form \( \tilde{a}_h(u_h, v_h) \) includes the face integrals only on the interior edges, whereas, the term \( J^2_h(u_h, v_h) \) includes the corresponding face integrals on the boundary edges and together with the right hand side \( I_h(v_h) \) changes depending on the boundary conditions. If Dirichlet boundary condition, \( u = g_D \), is prescribed, we set
\[
J^2_h(u, v) = - \sum_{E \in \mathcal{E}_1^h} \int_E \{\varepsilon^2 \nabla u\} \cdot [v] ds - \sum_{E \in \mathcal{E}_0^h} \int_E \{\varepsilon^2 \nabla v\} \cdot [u] ds + \sum_{E \in \mathcal{E}_1^h} \frac{\sigma\varepsilon^2}{h_E} \int_E [u] \cdot [v] ds,
\]
\[
I_h(v) = \sum_{E \in \mathcal{E}_0^h} \int_E \left( \frac{\sigma\varepsilon^2}{h_E} v - \varepsilon^2 \nabla v \cdot n \right) g_D ds.
\]

In the case of Neumann boundary condition, \( \varepsilon^2 \nabla u \cdot n = g_N \), they become
\[
J^2_h(u, v) = 0, \quad I_h(v) = \sum_{E \in \mathcal{E}_0^h} \int_E g_N vd s.
\]

When periodic boundary condition is applied, the periodic edges are treated as interior edges, in other words, as unknown with appropriate definitions of the so-called jump and average terms. In this case, the set of all edges \( E_h \) is splitted into the set \( E_0^h \) of interior edges and the set \( E_{per}^h \) of periodic boundary edge–pairs. An individual element of the set \( E_{per}^h \) is of the form \( \omega = \{E_l, E_m\} \) where \( E_l \subset \partial K_l \cap \partial \Omega \), and \( E_m \subset \partial K_m \cap \partial \Omega \) is the corresponding periodic edge-pair of \( E_l \) with \( l > m \), and we associate with each \( \omega \) a common normal vector \( n \) that is outward unit normal to \( E_l \subset \partial K_l \cap \partial \Omega \). Then, for each such \( \omega \), we define the jump and average operators
\[
[u]_\omega = u|_{E_l} n - u|_{E_m} n, \quad \{u\}_\omega = \frac{1}{2}(u|_{E_l} + u|_{E_m}).
\]
In this case, we have

\[
J_h^2(u, v) = - \sum_{\omega \in E_{\text{per}}} \int_{\omega} \left\{ e^2 \nabla u \right\}_\omega \cdot [v]_\omega ds - \sum_{\omega \in E_{\text{per}}} \int_{\omega} \left\{ e^2 \nabla v \right\}_\omega \cdot [u]_\omega ds
+ \sum_{\omega \in E_{\text{per}}} \frac{\sigma e^2}{h_E} \int_{\omega} [u]_\omega \cdot [v]_\omega ds,
\]

and \( I_h(v) = 0 \).

3 Time Discretization by Average Vector Field Method

The semi-discretized Allen-Cahn equation is a gradient system \( \dot{y} = -\nabla U(y) \) evolving into a state of minimal energy. They are characterized by the monotonically energy decreasing property of the potential

\[ U(y(t)) \leq U(y(s)), \quad \text{for} \ t > s. \]

In the numerical approximation of the gradient systems, it is desirable to preserve the energy decreasing property monotonically

\[ U(y(t_n)) \leq U(y(t_{n-1})), \quad \text{for} \ n = 1, 2, \cdots \]

The average vector field (AVF) method

\[ y_n = y_{n-1} - \Delta t \int_0^1 \nabla U(\tau y_n + (1 - \tau)y_{n-1}) d\tau \]

possesses the energy decreasing property without restriction to step sizes \( \Delta t \). It represents a modification of the implicit mid-point rule and for quadratic potentials \( U(y) \), the AVF reduces to the mid-point rule. Higher order variants of the AVF methods for Hamiltonian and Poisson systems with Gauss-Legendre collocation points are given in [13, 6]. As Gauss-Legendre Runge-Kutta methods, the AVF method and higher order versions do not have damping property for very stiff systems, whereas for discontinuous Galerkin-Petrov methods and Radua II Runge-Kutta methods, the energy decreases monotonically without restriction to the step size \( \Delta t \) and the Lipschitz constant for \( \nabla U(y) \). But they require solution of coupled system of equations, which increases the computation cost for 2 and 3 dimensional Allen-Cahn equations, where efficient solution techniques are required [9]. The AVF method can be regarded as an efficient integrator, when the nonlinearities are of polynomial type as for the Allen-Cahn equation, i.e. the integrals by the DG semi-discretized can be computed with the desired accuracy at low cost.

The AVF method is equivalent to the Petrov-Galerkin discontinuous Galerkin in time, when the trial functions are piecewise linear and the test functions are piecewise constant, which are given by

\[ y_n = y_{n-1} - \int_{t_{n-1}}^{t_n} \nabla U(\Delta t^{-1}(t - t_{n-1})y_n + \Delta t^{-1}(t_{n-1} - t)y_{n-1}) dt. \]


With the time parametrization \( t(\tau) = t_n - (t_n - t_{n-1}) \tau \) and using the change of variable formulation

\[
\int_{t_{n-1}}^{t_n} g(t) dt = \int_0^1 g(t(\tau)) \frac{dt(\tau)}{d\tau} d\tau,
\]

we obtain for the integral term in (7)

\[
y_n = y_{n-1} - \int_{t_{n-1}}^{t_n} \nabla U(\Delta t^{-1}(t - t_{n-1})y_n + \Delta t^{-1}(t_n - t)y_{n-1}) dt
\]

\[
= y_{n-1} - \Delta t \int_0^1 \nabla U(\tau y_n + (1 - \tau)y_{n-1}) d\tau
\]

which is the AVF method on the interval \([t_{n-1}, t_n]\).

We consider the SIPG semi-discretized system in the previous section

\[
(\partial_t u_h, v_h) + a_h(u_h, v_h) + (f(u_h), v_h) = I_h(v_h), \forall v_h \in V_h, t \in (0, T],
\]

with the time-dependent solution of the form

\[
u_h(t) = \sum_{m=1}^{N} \sum_{j=1}^{n_q} \xi_j^m(t) \phi_j^m
\]

where \( \phi_j^m \) and \( \xi_j^m \), \( j = 1, \ldots, n_q \), \( m = 1, \ldots, N \), are the basis functions of \( V_h \) and the unknown coefficients, respectively, with \( n_q \) is the local dimension such that \( n_q = q + 1 \) for 1D problems, \( n_q = \frac{(q+1)(q+2)}{2} \) for 2D problems, and \( N \) is the number of intervals for 1D problems or the number of triangular elements for 2D problems. Substituting (9) into (8) and choosing \( \nu = \phi_i^k \), \( i = 1, \ldots, n_q \), \( k = 1, \ldots, N \), we get the semi linear system of ordinary differential equations as a gradient system

\[
M \ddot{\xi}_i = -\nabla U(\dot{\xi}) = L - A \xi - b(\xi)
\]

for the ordered unknown coefficient vector

\( \dot{\xi} = (\dot{\xi}_1, \dot{\xi}_2, \ldots, \dot{\xi}_{n_q}, \xi_1^1, \xi_1^2, \ldots, \xi_{n_q}^1, \xi_1^2, \ldots, \xi_{n_q}^2, \ldots, \xi_1^N, \ldots, \xi_{n_q}^N)^T \), same order for the basis functions, where \( M \) is the mass matrix with the entries \( M_{ij} = (\phi_i^j, \phi_i^j) \), \( 1 \leq i, j \leq n_q \times N \), \( A \) is the stiffness matrix with the entries \( A_{ij} = a_h(\phi_i^j, \phi_i^j), 1 \leq i, j \leq n_q \times N \), \( b \) is the non-linear vector of unknown coefficient vector \( \dot{\xi} \) with the entries \( b_i(\dot{\xi}) = (f(u_h), \phi_i^k) \), \( 1 \leq i \leq n_q \times N \), and \( L \) is the load vector \( i-th \) component of which corresponding to the right hand side linear form \( I_h(\phi^i) \), \( 1 \leq i \leq n_q \times N \).

We consider the uniform partition \( 0 = t_0 < t_1 < \ldots < t_J = T \) of the time interval \([0, T]\) with the uniform time step-size \( \Delta t = t_k - t_{k-1}, k = 1, 2, \ldots, J \). For \( t = 0 \), let \( u_h(0) \in V_h \) be the projection (orthogonal \( L^2 \)-projection) of the initial condition \( u_0 \) onto \( V_h \), and let \( \xi_0 \) be the corresponding coefficient vector (ordered) satisfying (9). Then, the average vector field method applied to the gradient system (10) reads as:
for \( n = 0, 1, \ldots, J - 1 \), solve

\[
\frac{M_{\xi_{n+1}} - M_{\xi_n}}{\Delta t} = - \int_0^1 \nabla U(\tau \xi_{n+1} + (1 - \tau) \xi_n) d\tau
\]

\[
M_{\xi_{n+1}} = M_{\xi_n} + \Delta t \int_0^1 [L - A(\tau \xi_{n+1} + (1 - \tau) \xi_n)] d\tau
\]

After a simple calculation for the linear part, we get

\[
M_{\xi_{n+1}} = M_{\xi_n} + \Delta t L - \Delta t \left( \frac{A_{\xi}}{2} + A_{\xi_{n+1}} \right) - \Delta t \int_0^1 b(\tau \xi_{n+1} + (1 - \tau) \xi_n) d\tau
\]

which is the fully discretized system that we will solve for \( \xi_{n+1} \). We solve this nonlinear system of equations using Newton’s method. From the algebraic point of view, Newton’s method for (11) corresponds to solving the nonlinear equations

\[
R(\xi_{n+1}) = M_{\xi_{n+1}} - M_{\xi_n} - \Delta t L - \Delta t \left( \frac{A_{\xi}}{2} + A_{\xi_{n+1}} \right) + \Delta t \int_0^1 b(\tau \xi_{n+1} + (1 - \tau) \xi_n) d\tau = 0.
\]

Starting with an initial guess \( \xi_{n+1}^{(0)} \), the \( k\)th Newton iteration to solve the nonlinear equation (12) for the unknown vector \( \xi_{n+1} \) reads as

\[
J_s^{(k)} = -R(\xi_{n+1}^{(k)}), \quad \xi_{n+1}^{(k+1)} = \xi_{n+1}^{(k)} + s^{(k)}, \quad k = 0, 1, \ldots
\]

until a user defined tolerance is satisfied. In (12), \( J \) stands for the Jacobian matrix of \( R(\xi_{n+1}) \), whose entries are the partial derivatives

\[
J_{ij} = \frac{\partial R_i}{\partial (\xi_{n+1})_j}, \quad i, j = 1, 2, \ldots, n_y \times N
\]

at the current iteration. It is easy to differentiate the linear terms in (12)

\[
\frac{\partial}{\partial (\xi_{n+1})_j} (M_{\xi_{n+1}} - M_{\xi_n} - \Delta t L + \Delta t \left( \frac{A_{\xi}}{2} + A_{\xi_{n+1}} \right)) = M_{ij} + \Delta t \frac{A_{ij}}{2}.
\]

We apply the chain rule to differentiate the nonlinear term,

\[
\frac{\partial}{\partial (\xi_{n+1})_j} \int_0^1 b(\tau \xi_{n+1} + (1 - \tau) \xi_n) d\tau = \Delta t \int_0^1 \frac{\partial}{\partial (\xi_{n+1})_j} (b(\tau \xi_{n+1} + (1 - \tau) \xi_n)) d\tau
\]

\[
= \Delta t \int_0^1 \frac{\partial}{\partial (\xi_{n+1})_j} (\tau \frac{\partial b}{\partial (\xi_{n+1})_j}) (\tau \xi_{n+1} + (1 - \tau) \xi_n) d\tau
\]
where, using the expansion \( u_h = \sum_{k=1}^{n_N} \xi_k \phi^k \), ordered version of (9),

\[
\frac{\partial b_i(\xi)}{\partial \xi_j} = \frac{\partial}{\partial \xi_j} (f(u_h), \phi^i) = \int_{\Omega} f'(u_h) \phi^i \phi^j \, dx
\]

(13)

where \( f(u) = u^3 - u \) and \( f'(u) = 3u^2 - 1 \) in our model. Hence, we obtain that

\[
J = M + \frac{\Delta t}{2} A + \Delta t \int_0^1 \tau J_b(\tau \xi_{n+1}^{(k+1)} + (1 - \tau) \xi_n) \, d\tau
\]

(14)

where \( J_b(\tau \xi_{n+1}^{(k+1)} + (1 - \tau) \xi_n) \) is the differential matrix, whose entries are given in (13), at \( \tau \xi_{n+1}^{(k+1)} + (1 - \tau) \xi_n \). At each Newton iteration, we approximate the integral term in (14) using fourth order Gaussian quadrature rule.

4 Numerical Results

In all numerical experiments, we have used for the space discretization linear elements. Only for the ripening time calculations, linear and quadratic elements are used for comparison.

4.1 1D Allen–Cahn with Neumann boundary condition

Our first problem is 1D Allen–Cahn equation with homogeneous Neumann boundary conditions in the domain \((x,t) \in [-1,1] \times [0,80]\) and with the initial condition [4]

\[
\frac{\partial u}{\partial x}(-1,t) = \frac{\partial u}{\partial x}(1,t) = 0, \quad u(x,0) = 0.53x + 0.47\sin(-1.5\pi x),
\]

The parameter \( \varepsilon^2 = 0.01 \) is taken as in [4], where in [4] the Allen Cahn equation is discretized in space by Fourier spectral elements and Strang splitting is used for time discretization with the mesh sizes \( \Delta x = \Delta t = 0.02 \). We have taken the mesh sizes as \( \Delta x = \Delta t = 0.01 \). The evolution of phase function and energy are given in Figure 1. Allen-Cahn equation has one stable, \( u = 0 \), and two unstable, \( u = \pm 1 \), equilibria, whereas the solutions move from one equilibrium to the other one, which is known as phase separation. The interfaces between two unstable equilibria move over exponentially long times between the region, which is known as metastability phenomenon. The phase separation, right plot in Figure 1, shows the metastable state clearly. The state of phase function is reflected in monotonically decreasing numerical energy, left plot in Figure 1.

4.2 1D Allen–Cahn with periodic boundary condition

We consider the 1D Allen–Cahn problem with periodic initial and boundary conditions with diffusion constant \( \varepsilon = 0.12 \) [22] in the domain \((x,t) \in [0,2\pi] \times [0,600]\)

\[
u(0,t) = u(2\pi,t), \quad u_s(0,t) = u_s(2\pi,t), \quad u(x,0) = 0.8 + \sin(x)
\]
Computations are done with the step sizes $\Delta x = \pi/50$ and $\Delta t = 0.01$. The same problem was solved in [22] again using Fourier spectral space discretization with the mesh size $\Delta x = \pi/64$ and with adaptive time integration using Backward Differential formula (BDF3)- Adams-Bashfort method (AB-3).

We see Figure 2 the fast dynamics from the initial condition to the metastable state, where two transition layers are formed. Also, the numerical energy is decreasing monotonically.

4.3 Time adaptivity with AVF and ripening time

The transition layers of the Allen-Cahn equation move quickly from one unstable equilibrium to the other one by crossing the zero axis. The time where the solution takes its minimum value is named as the ripening time. The ripening time is computed for the Allen-Cahn equation with periodic boundary conditions using adaptive time stepping in [22, 5]. For the construction of adaptive time grids, one needs a local error estimator. For local error estimation, two discrete solutions $u_\tau$, $\hat{u}_\tau$ of order $p + 1$ and $p$ are computed in parallel such that

$$u_\tau(\tau) = u(\tau) + O(\tau^{p+2}), \quad \hat{u}_\tau(\tau) = u(\tau) + O(\tau^{p+1}).$$
with \( \tau \) denoting the time step size \( \Delta t \). Then

\[
\hat{\varepsilon}_\tau = \| u_\tau(\tau) - \hat{u}_\tau \| = C\tau^{p+1}
\]

(15)
is an estimator of the actual \( \hat{\varepsilon}_\tau \) of \( \hat{u}_\tau \) measured in an Euclidean norm [7]. We search for an optimal step size \( \tau^* \), for which \( \hat{\varepsilon}_{\tau^*} \leq \delta_{TOL} \), where \( \delta_{TOL} \) denotes a user specified tolerance. By insertion of both \( \tau \) and \( \tau^* \) into (15), we arrive at the estimation formula

\[
\tau^* = p+1 \sqrt{\frac{p\delta_{TOL}}{\hat{\varepsilon}_\tau}}
\]

with a safety factor \( \rho \approx 0.9 \). If \( \hat{\varepsilon}_{\tau^*} \leq \delta_{TOL} \), then the presented step size \( \tau^* \) is accepted and \( \tau^* \) is used in the next step; otherwise the present step size is rejected and the current step is repeated with the step size \( \tau^* \). In the successful case, the more accurate value \( u_\tau(\tau) \) will be used to start the next step. For the adaptive time stepping scheme, we choose backward Euler method and average vector field method which are of order \( p \) and \( p+1 \), respectively, with \( p = 1 \). As initial time step size \( \tau = 0.05 \) is taken.

For the ripening time estimates, the number of time steps are expected to increase linearly by decreasing tolerances \( \delta_{TOL} \) with the ratio \( \frac{M(\delta_{TOL}/10)}{M(\delta_{TOL})} = \rho\sqrt{10} \), where the order of the method is \( p = 1 \). Table 1 shows the ripening time for 1D Allen–Cahn equation with periodic boundary condition (Example 4.2) for linear and quadratic polynomials. We see that our solution converges to \( T_r = 546.5 \).

<table>
<thead>
<tr>
<th>( \delta_{TOL} )</th>
<th>Ripening Time</th>
<th># Time Steps</th>
<th>( M(\delta_{TOL}^p)/M(\delta_{TOL}^{p-1}) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1e-04</td>
<td>549.52 (539.71)</td>
<td>480 (480)</td>
<td>3.02 (3.02)</td>
</tr>
<tr>
<td>1e-05</td>
<td>554.46 (544.54)</td>
<td>1515 (1515)</td>
<td>3.12 (3.16)</td>
</tr>
<tr>
<td>1e-06</td>
<td>555.99 (546.05)</td>
<td>4792 (4790)</td>
<td>3.16 (3.16)</td>
</tr>
<tr>
<td>1e-07</td>
<td>556.47 (546.52)</td>
<td>15153 (15152)</td>
<td>3.16 (3.16)</td>
</tr>
</tbody>
</table>

Table 1: Example 4.2: Convergence of the ripening time with the adaptive AVF method using linear (quadratic) polynomials.

![Time-Steps vs Time](image)
4.4 2D Allen–Cahn with periodic boundary condition

2D Allen–Cahn equation under periodic initial and boundary conditions for the diffusion constant $\epsilon = 0.18$ in [22] in the domain $(x,y,t) \in [0,2\pi]^2 \times [0,33]$ is given as:

$$u(x,y,0) = 2e^{\sin(x)+\sin(y)-2} + 2.2e^{-\sin(x)-\sin(y)-2} + 1,$$

$$u(0,t) = u(2\pi,t) \quad \text{and} \quad u_x(0,t) = u_x(2\pi,t), \quad u_y(0,t) = u_y(2\pi,t).$$

We have taken as mesh size $\Delta x = \Delta y = \pi/8$ after three refinement steps in order to obtain accurate solutions. The solutions with contour plots for uniform time integration with the step size $\Delta t = 0.01$ for the initial and final time are shown in Figure 4. It is observed that the smaller region is annihilated prior to the larger region. Both reach the stable state of $u = -1$ at the end as we expect.

Figure 4: Example 4.4: The evolution of phase functions for the step-size $\Delta t = 0.01$.

The ripening time for different tolerances with linear and quadratic polynomials is given in Table 2. We observe that the ripening time converges by decreasing tolerance and the ratio is close to the theoretical one 3.3. The numerical energy is also decreasing for the adaptive time stepping in Figure 5, as for the Allen-Cahn and Cahn-Hilliard equations in [22, 5].

4.5 2D Allen–Cahn with Dirichlet boundary conditions

We consider 2D Allen–Cahn equation with homogenous Dirichlet boundary condition [12]. The initial condition is randomly distributed from $-0.01$ to $0.01$ to
Figure 5: Example 4.4: Decay of the numerical energy (left) and the evolution of time steps (right) using linear polynomials for \( \delta_{TOL} = 1 \times 10^{-4} \).

<table>
<thead>
<tr>
<th>( \delta_{TOL} )</th>
<th>Ripening Time</th>
<th># Time Steps</th>
<th>( M(\delta_{TOL}^n)/M(\delta_{TOL}^{n-1}) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1e-03</td>
<td>27.20 (30.10)</td>
<td>209 (216)</td>
<td>3.12 (3.13)</td>
</tr>
<tr>
<td>1e-04</td>
<td>27.33 (30.24)</td>
<td>668 (692)</td>
<td>3.20 (3.20)</td>
</tr>
<tr>
<td>1e-05</td>
<td>27.37 (30.25)</td>
<td>2121 (2197)</td>
<td>3.18 (3.17)</td>
</tr>
<tr>
<td>1e-06</td>
<td>27.37 (30.27)</td>
<td>6707 (6956)</td>
<td>3.16 (3.17)</td>
</tr>
</tbody>
</table>

Table 2: Example 4.4: Convergence of the ripening time with adaptive AVF method using linear (quadratic) polynomials.

Each grid point. We take \( \varepsilon = 0.01, \Delta x = \Delta y = \pi/8 \) and \( \Delta t = 0.1 \), and the domain \( \Omega = [0, 2\pi] \times [0, 2\pi] \). In Figure 6, the corresponding solution contours are plotted, the numerical energy is decreasing again monotonically.

Figure 6: Example 4.5: Evolution of phase functions at different times.
5 Conclusions

We have presented numerical results for Allen–Cahn equation under periodic, Neumann and Dirichlet boundary conditions using DGFEM discretization in space and energy stable AVF method in time. The numerical energy is decreasing in all examples and the numerical solutions are similar to those in the literature. We have shown that the ripening time can be detected correctly and the metastability phenomena can be observed numerically. Because the DG method is suitable for handling sharp interfaces and singularities due to its local nature, in a future work we will study adaptive DGFEM methods for the sharp interface limit ($\varepsilon \to 0$) of the Allen-Cahn equation (see for example [24]).

6 Acknowledgements

This work has been supported by Scientific HR Development Program (OYP).

References


