Explicit Runge-Kutta scheme with high efficiency and energy dissipation for the Allen-Cahn equation

Ke Li$^{1,a}$, Huan Zhang$^2$

$^1$College of Liberal Arts and Sciences, National University of Defense Technology, Changsha 410073, China;
$^1$Email: 643275623@qq.com

$^2$The 63768 Troop of The People’s Liberation Army of China, Xian, 710600, China;
$^2$Email: 937314751@qq.com

Abstract. This paper presents a series of explicit Runge-Kutta solution to the Allen-Cahn equation, using the same energy and the square of the newly developed method were analyzed. Based on the explicit Runge-Kutta, we find that these schemes not only have high accuracy, high-order convergence and efficiency, but also have energy-consuming characteristics. We first convert the nonlinear Allen-Cahn equation into an equivalent equation that satisfies the law of quadratic energy dissipation. Then, we discretize the reconstruction by using the Runge-Kutta scheme in the time direction. Theoretical analysis and numerical simulation results verify the algorithm’s dissipation characteristics, convergence order and long-term simulation stability.

1. Introduction
Allen and Cahn [1], in order to explain the movement of an amorphous solid by reverse phase boundaries, proposed Allen-Cahn equation. Today Allen-Cahn equation is the phase field model that is most widely used for a number of physical phenomena in materials science and fluid mechanics. Start in a one-dimensional Allen-Cahn equation, such as the following.

\[ u_t = \varepsilon^2 \Delta u - f'(u), \]  

where \( f(u) = \frac{1}{4} (u^2 - 1)^2 \) and \( \varepsilon \) are constant parameters of the actual, on the basis of the following initial and periodic boundary conditions

\[ u(x, 0) = u_0(x), x \in \Omega = [c, d], \]  
\[ u(c, t) = u(d, t), t \geq 0, \]

Under the periodic boundary conditions, the general energy of Allen-Cahn equation is as follows.

\[ E(u) = \int_\Omega \frac{\varepsilon^2}{2} |\nabla u|^2 + f(u) dx. \]  

Then the above equation (1) can be written as

\[ u_t = -m, \]
\[
m = \frac{dE(u)}{du} = -\varepsilon^2 \Delta u + f'(u).
\] (6)

The following is inner product of the (5) with \( m \) and the (6) with \( u_t \),
\[
\frac{d}{dt} E(u) = -\langle m, m \rangle \leq 0.
\] (7)

Thus, the Allen-Cahn equation conforms to the law of energy dissipation.

The Allen-Chan equation has many numerical techniques being developed. One of the common schemes is the convex splitting method, which was first proposed by Elliott and Stuart in 1993 [1]. The numerical energy stability is achieved and was further studied by Eyre [3]. This scheme not only implicitly deals with the convex part of the chemical potential but also the concave part, thus obtaining the unique solvability and energy stability.

The invariant energy quadratization (IEQ) method is a recently expanded technology that second-order invariant conservation allows you to preserve the laws that preserve polynomial structures of degree. The general idea of IEQ is to change the original equation from a variable system with higher-order energy terms to an similar coupled system, according to the original energy formulation [4, 5, 6, 7, 8, 9, 10, 11]. In this article, we focused on one-dimensional Allen-Cahn equation, by applying explicit Runge-Kutta methods in the time direction and a Fourier Pseudospectral scheme used in the spatial direction, a series dissipative approach to discrete reformulated Allen-Cahn system.

Other chapters of this article are arranged as follows. In Section 2, by using the invariant energy quadratization approach, introducing an equivalent system with energy dissipation theorem. In Section 3, introducing the Fourier pseudospectral method in the spatial semi-discrete system, using the explicit Runge-Kutta schemes which are high order and dissipative in Section 4. Both of the semi-discrete and fully discrete systems are rigorously proven energy dissipating in corresponding sections. In the last section, numerical experiments for 1D cases are demonstrated to verify the dissipative properties.

2. Energy dissipative scheme using the IEQ approach

The domain \( \Omega \) with a smooth boundary. The \( L^2 \) inner product are defined as \( \langle u, v \rangle = \int_{\Omega} uv dx \) and
\[
\|u\|_2 = \sqrt{\langle u, u \rangle}, \quad \forall u, v \in L^2(\Omega).
\]
By introducing an auxiliary variable \( r(u) = f(u) + c_0 \), where \( c_0 \) is a constant that ensures the term under square root is positive. In this passage, we set \( c_0 = 0 \). The Allen-Cahn equation (5) (6) can be transformed into
\[
\begin{align*}
u_t &= \varepsilon^2 \Delta u - 2rr_u, \\
r_t &= \frac{f'(u)}{2r} u_t,
\end{align*}
\] (8) (9)

**Theorem 2.1.** The system (8)-(9) benefit from the following energy dissipation law
\[
\frac{d}{dt} E(u) = \frac{d}{dt} \left( \int_{\Omega} \frac{\varepsilon^2}{2} |\nabla u|^2 + r^2 dx \right) \leq 0.
\] (10)

**Proof.** The system (8)-(9) can be written as
\[
\begin{align*}
u_t &= -m, \\
m &= -\varepsilon^2 \Delta u + 2rr_u, \\
r_t &= \frac{f'(u)}{2r} u_t.
\end{align*}
\] (11) (12) (13)

By taking the inner products of the (11)-(13) with \( m, u_t, r_t \), respectively, we gain the following equalities
\[ \langle u, m \rangle = \langle -m, m \rangle, \quad (14) \]
\[ \langle m, u \rangle = \langle -\varepsilon^2 \Delta u + 2rr_u, u \rangle, \quad (15) \]
\[ \begin{bmatrix} r \cr r \end{bmatrix} = \begin{bmatrix} f'(u) \cr 2r_u \end{bmatrix}, \quad (16) \]

By substituting equation (15)-(16) into equation (14), we obtain
\[ \frac{d}{dt} E(u) = \frac{d}{dt} \left( \int_{\Omega} \frac{\varepsilon^2}{2} |\nabla u|^2 + r^2 \, dx \right) = -\langle m, m \rangle \leq 0. \quad (17) \]

the proof is complete.■

Let \( z = (u, r)^T \), the equation (8)-(9) can be expressed as
\[ z_t = F(z). \quad (18) \]

Under the periodic boundary conditions, the equation (8)-(9) admit the dissipative energy
\[ E(z) = \langle Sz, z \rangle_{\Omega} = \int_{\Omega} z^T S z \, dx = \int_{\Omega} \frac{\varepsilon^2}{2} |\nabla u|^2 + r^2 \, dx, \quad (19) \]

3. **Energy dissipative spatial semi-discretization using the Fourier pseudospectral method**

For discretize equation (8) and (9) in a spatial direction, we use the effective Fourier pseudospectral method. The essential to the Fourier pseudospectral method is to be similar to the partial differential operators. Ref.[12] introduces the Fourier spectral differential matrix \( D_k \) can be similar to the \( k \)-th order partial differential operator \( \partial^k \) with spectral accuracy. We express \( D_1 \) as follows:
\[ (D_{m+1,n+1}) = \begin{cases} \frac{1}{2} (-1)^{m+n} \mu \cot \left( \frac{\mu (X_n - X_m)}{2} \right), & m \neq n, \\ 0, & m = n, \end{cases} \]

where \( \mu = \frac{2\pi}{L} \), \( L \) is the distance of spatial interval and the integer \( N \) is also the number of sub-intervals, \( h = \frac{L}{N} \) is evident, \( D_1 \) is an \( N \times N \) real skew-symmetric matrix. For more details, see Ref.[13] and references therein.

We obtain the semi-discrete system
\[ u_t = \varepsilon^2 D_1 u_t - 2rr_u, \quad (20) \]
\[ r_t = \frac{f'(u)}{2}r_u, \quad (21) \]

where \( r = [r_0, r_1, \ldots, r_{N-1}]^T \), \( u = [u_0, u_1, \ldots, u_{N-1}]^T \) and \( u \cdot r = [u_0r_0, u_1r_1, \ldots, u_{N-1}r_{N-1}]^T \).

Next, we will show that this system possesses a semi-discrete modified energy dissipation law.

**Theorem 3.1** The semi-discrete equation (22)-(23) have the semi-discrete corrected energy dissipation law:
\[ \frac{d}{dt} E(u, r) = \frac{d}{dt} \left( \int_{\Omega} \frac{\varepsilon^2}{2} |D_1 u|^2 + r^2 \, dx \right) \leq 0, \quad (22) \]

where \( E(u) = \frac{\varepsilon^2}{2} \|D_1 u\|^2 + \sum_{i=1}^{N-1} r_i^2 \).

**Proof.** The equation (22)- (23) can be written as
\[ u_i = -m, \]  
\[ m = -\varepsilon^2 D_i^2 u + 2 \varepsilon r_i, \]  
\[ r_i = \frac{f'(u)}{2 \varepsilon} u_i. \]  

By taking the inner product of the system (25)-(27) with \( u_i, m \), and \( \frac{r_i}{2} \), respectively, we have following energy dissipation

\[
\frac{d}{dt} E(u, r) = \frac{d}{dt} \left( \frac{\varepsilon^2}{2} \| D_i u \|^2 + \sum_{i=1}^{n} r_i^2 \right) = -\langle m, m \rangle \leq 0. \tag{26}
\]

the proof is complete. ■

4. High order dissipative explicit IEQ-RK method

In this section, by applying the technique of invariant energy quadratization, a kind of explicit Runge-Kutta with high order energy dissipative schemes are presented. We first recall the s-stage RK scheme.

S-stage RK scheme: The \( \Delta t \) denotes the time step, \( t_n = n \Delta t \), \( u^n \) and \( r^n \) stand for the numerical solution for \( u \) and \( r \) on time \( t_n \). For given \( z^n = z(t_n) \), when s-stage RK method is applied to the equation (1), the following intermediate values are first calculated by

\[
z_i = z^n + \Delta t \sum_{j=1}^{s} a_{ij} F_j, \tag{27}
\]

where \( F_j = F(z_j) \). Then \( z^{n+1} \) is updated in

\[
z^{n+1} = z^n + \Delta t \sum_{j=1}^{s} a_{nj} F_j. \tag{28}
\]

**Proposition 4.1** Runge-Kutta’s Butcher table

\[
\begin{array}{c|cccc}
c & a_{11} & a_{21} & \cdots & a_{s1} \\
\hline
b_1 & c_1 & a_{12} & \cdots & a_{s2} \\
\vdots & \vdots & \ddots & \ddots & \vdots \\
\hline
b_s & c_s & a_{1s} & \cdots & a_{ss} \\
\end{array}
\]

where \( c_i = \sum_{j=1}^{s} a_{ij}, \) and \( a_{ij} = 0(i < j), b_i \neq 0(i = 1, 2, \cdots, s). \)

Here, we only provide a proof of the energy and mass dissipation characteristics of a one-dimensional discrete system. However, readers will find it simple to generalize these proofs to 2D situations.

5. Numerical experiment

We consider the Allen-Cahn equation with the zero Neumann boundary condition, the following initial condition of the domain \( \Omega = [0, 1] \):

\[
u(x, 0) = 0.01 \cos(\pi x) + 0.25 \cos(4\pi x) + 0.2 \cos(11\pi x). \tag{29}
\]

For the numerical simulations, \( \varepsilon = 0.01 \) is utilized and fixed mesh size to \( \Delta x = 1/128 \) which gives enough space accuracy. Numerical solutions evolve over time \( T = 4 \).
Because there is no exact solution, so compute one reference solution \( u_{\text{ref}} \) by choosing \( \Delta t = 10^{-5} \) and \( \Delta x = 1/128 \).

Firstly, the profiles and the top view of numerical solution had by two Runge-Kutta schemes are demonstrated in Fig. 1 and Fig. 2, respectively. As examples, along with the real solution for comparison. The results show that two IEQ-RK programs simulate equation (1)-(3) accurately. Color of Fig. 2 reference Fig. 1.

Secondly, choosing the time steps \( \Delta t = 0.05, 0.025, 0.0125, 0.00625, 0.003125 \), the corresponding errors measured by \( \| z(t_n) - z^n \| \) and IEQ-RK of convergence rateschemes are presented in Table 1, the numerical convergence orders of IEQ-DIRK schemes agree with the theoretical orders.

![Figure 1: The profiles of numerical solutions of reference solution, IEQ-RK(2,2) and IEQ-RK(4,4).](image1)

![Figure 2: The top view of numerical solution obtained by reference solution, IEQ-RK(2,2) and IEQ-DT(4,4) at \( T = 5 \).](image2)

![Figure 3: The evolution of energy in three Runge-Kutta schemes at \( T = 10, \Delta t = 0.05 \).](image3)

![Figure 4: The evolution of errors of quadratic energy in three Runge-Kutta schemes at \( T = 10 \).](image4)
Finally, the evolution of energy of different stages IEQ-RK schemes are presented in Fig.3, we find the proposed scheme (8-9) with different stage IEQ-RK schemes can accurately retain discrete energy dissipation. The results show that the new scheme (8-9) can keep the proposed Allen-Cahn energy dissipation. The energy errors of different stages IEQ-RK schemes are presented in Fig.4, the evolution of the measured error be introduced by $\left|z_{t=f}^{\text{ref}}-z_{t}^{n}\right|$ for the quadratic invariants energy in the time interval $t \in [0,10]$. Comparatively speaking, it’s clear that IEQ-RK(4,4) are more accurate than other two schemes.

Table 1. $L^2$ errors and corresponding convergence orders at $T=4$

| RK(Stage, Order) | $\Delta t$ | IEQ-RK $L^2$ error | order |
|------------------|------------|---------------------|-------|
| RK(2,2)          | 0.05       | 1.666e-04           |       |
|                  | 0.025      | 4.215e-05           | 1.993 |
|                  | 0.0125     | 1.055e-06           | 1.997 |
|                  | 0.00625    | 2.596e-06           | 2.023 |
|                  | 0.003125   | 5.988e-07           | 2.116 |
| RK(3,3)          | 0.05       | 2.177e-06           |       |
|                  | 0.025      | 2.763e-07           | 2.978 |
|                  | 0.0125     | 3.479e-08           | 2.989 |
|                  | 0.00625    | 4.351e-09           | 2.996 |
|                  | 0.003125   | 5.292e-10           | 3.039 |
| RK(4,4)          | 0.05       | 2.562e-08           |       |
|                  | 0.025      | 1.594e-09           | 4.005 |
|                  | 0.0125     | 9.953e-10           | 4.002 |
|                  | 0.00625    | 6.213e-12           | 4.001 |
|                  | 0.003125   | 3.849e-13           | 4.012 |

6. Conclusion

In this article, we have studied the explicit Runge-Kutta method for the second-order energy dissipation of the Allen-Cahn equation. By using the invariant energy quadratization technique, we constructed a dissipative structure that satisfies the Allen-Cahn equation. According to this experimental design, the high efficiency, high-order convergence and dissipation characteristics of this scheme are proved by a series of numerical experiments.

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