Error analysis in unconditionally stable coarsening algorithms

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Abstract

In order to quantitatively study the accuracy of the unconditionally stable coarsening algorithms, we calculate the Fourier space multi step error on the order parameter field by explicitly distinguishing the analytic time $\tau$ and the algorithmic time $t$. The calculation determines the error in the order parameter and the scaled correlations. This error contributes a correction term in the analytic time step, which is crucial in understanding the accuracy in unconditionally stable coarsening algorithms.

Key words: Unconditionally stable, Error analysis, Algorithmic time step, Multi step error, Coarsening

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1 Introduction

The Partial Differential Equations (PDEs) that governs conserved and non-conserved scalar coarsening systems are the Cahn-Hilliard (CH) [1] and Allen-Cahn (AC) equations [2] respectively. Examples are found in polymer mixtures [3], alloys [4,5], liquid-crystals [6,7], and in cosmology [8]. These equations, as well as their various extended forms, are an active area of research. They model the phase separation that occurs after a quench from a high temperature disordered phase into two distinct phases at low temperatures. The pattern of the two phase regions coarsens as the time increases, i.e., the length-scale of these regions grows. The scaled correlation is an important probe to characterize the late time scaling regime, where the dynamics are dominated by a single

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length scale, the average domain size \( L \), which increases with a power law in time \( \tau \), \( L(\tau) \sim \tau^\alpha \) [9]. For the scalar order parameter systems considered in this paper, \( \alpha = 1/3 \) and \( 1/2 \) for conserved and non-conserved systems, respectively [9]. To study the coarsening systems, one needs to choose a random initial condition, which corresponds to a high temperature disordered phase. Since it is essentially not possible to find an exact solution for random initial conditions, computer simulation plays an important role in understanding these systems.

Because of the nature of slow coarsening process in the late time scaling regime, the main challenge in computer simulation of coarsening systems is to develop an efficient algorithm. The most straightforward approach is the Euler algorithm, which must employ a time step \( \Delta t_{Eu} \sim (\Delta x)^4 \) and \( (\Delta x)^2 \) to maintain stability for conserved and non-conserved systems, respectively, where \( \Delta x \) is the lattice spacing. On the other hand, one has to use a lattice spacing \( \Delta x < \xi \) to resolve the interfacial profile, where \( \xi \) is the interfacial width. This implies that the Euler update is inefficient, and in practice computationally costly to use to evolve large systems until the late time scaling regime. Various computational algorithms have been developed by increasing the algorithmic time step \( \Delta t \) compared to the simplest Euler discretization. For example, the Cell Dynamical System (CDS) [10–12] was broadly applied [13,14] as an efficient technique. However, a transformation of CDS to PDE [15,16] showed that CDS changes the form of the equation of motion within the same universality class and gets a less strict stability threshold for its Euler update, but the Euler time step is still limited to \( (\Delta x)^4 \) and \( (\Delta x)^2 \) for conserved and non-conserved systems, respectively. More recently, conditionally stable algorithms such as Fourier spectral methods [17,18] have been developed by introducing implicit terms in the update equation, and have been shown to allow an increase of the algorithmic time step \( \Delta t \) by two orders of magnitude. However, none of these methods can adjust to the naturally slowing dynamics - they eventually become more and more inefficient at the late time scaling regime.

The recently developed unconditionally stable algorithms [19–21] overcomes the difficulty of a fixed time step for maintaining stability and allows for arbitrarily large algorithmic time steps. In CH equation, the algorithm allows an optimal driving scheme \( \Delta t = A \tau^{2/3} \) with the error in correlations scales as \( \sqrt{A} \) for small prefactor \( A \) [22,23]. This implies that any driving scheme that is slower than the optimal one is wastefully accurate because the error is negligible in correlations [23]. This algorithm has also been applied to other interesting systems, such as the Phase Field Crystal (PFC) model [24,25] and the Swift-Hohenberg (SH) equation and showed significantly improved efficiency [26].

While we have no doubt about the efficiency of unconditionally stable algorithms, the accuracy of unconditionally stable algorithm, remains somewhat
mysterious, and some open questions remain unanswered. For example, why does the single step error accumulate over time [22,23]? why does the fitting for the maximal analytic time step in non-conserved system get worse as $\tilde{a}$ [see Eq. (24) for a precise definition] increases? In this paper, by explicitly calculating the Fourier space multi step error using Eq. (15), we are able to answer these questions. The rest of the paper is organized as follows. In Section 2, we briefly review the results in the previous work [19–23] and introduces the basic concepts and notations of unconditionally stable algorithms. In Section 3, we study the Fourier space multi step error, where the distinction of the analytic time and the algorithmic time is necessary. Based on this result, in Section 4, we determine the accuracy in the scaled structure factor $g(x)$ and $h(x)$. We then calculate the analytic time step in Section 5, taking into account the error in $h(x)$. The summary are presented in Section 6. In the appendix, we derive the scaling of field derivatives for all modes in Fourier space. For simplicity but without loss of generality, we restrict our analysis to two dimensions (2D).

2 Review of Unconditionally stable algorithms

For coarsening systems, a suitable free energy functional to describe the ordered phase is [9]

$$F[\phi] = \int d^2 x \left[ \frac{1}{2} |\nabla \phi|^2 + V(\phi) \right],$$  

(1)

where $\phi(x, t)$ is the order parameter, and the potential $V(\phi)$ has a double-well structure $V(\phi) = (\phi^2 - 1)^2/4$. The two minima of $V$ correspond to the two equilibrium phases $\phi = \pm 1$. The term $V(\phi)$ describes the energy in the bulk. The gradient-squared term in Eq. (1) associates an energy cost to an interface between the two phases.

When the order parameter is conserved under the dynamics, the equation of motion can be written in the form of a continuity equation, $\partial \phi / \partial t = -\nabla \cdot j$, with current $j = -M \nabla (\delta F / \delta \phi)$, where $M$ is the mobility. Absorbing $M$ into the time scale, we obtain the dimensionless form of Cahn-Hilliard (CH) equation [1]:

$$\frac{\partial \phi}{\partial \tau} = \nabla^2 \frac{\delta F}{\delta \phi} = -\nabla^2 (\nabla^2 \phi + \phi - \phi^3).$$  

(2)

In the case where the order parameter is not conserved by the dynamics, the simplest dissipative equation for the time evolution of the field $\phi$ is
\[
\frac{\partial \phi}{\partial \tau} = -\frac{\delta F}{\delta \phi} = \nabla^2 \phi + \phi - \phi^3. \tag{3}
\]

Eq. (3) describes that the rate of change of \( \phi \) is proportional to the gradient of the free-energy functional in functional space, and is often called the Allen-Cahn (AC) equation [2].

In order to obtain unconditionally stable algorithms for these equations, we introduce a mix of explicit and implicit terms in the update [19–21]. For the CH equation, we have

\[
\phi_{t+\Delta t} - (a_1 - 1)\Delta t \nabla^2 \phi_{t+\Delta t} - (a_2 - 1)\Delta t \nabla^4 \phi_{t+\Delta t} = \phi_t - \Delta t(a_1 \nabla^2 \phi_t + a_2 \nabla^4 \phi_t - \nabla^2 \phi^3_t), \tag{4}
\]

and for the AC equation, we have

\[
\phi_{t+\Delta t} + (a_1 - 1)\Delta t \phi_{t+\Delta t} + (a_2 - 1)\Delta t \nabla^2 \phi_{t+\Delta t} = \phi_t + \Delta t(a_1 \phi_t + a_2 \nabla^2 \phi_t - \phi^3_t). \tag{5}
\]

Implicit terms \((\phi_{t+\Delta t})\) are on the left and the explicit terms \((\phi_t)\) are on the right. Unconditionally stable algorithms are obtained for \(a_1 > 2\) and \(a_2 < 1/2\) [19–21]. In Fourier space, Eq. (4) can be directly solved as

\[
\phi_k(t + \Delta t) = \phi_k(t) + \Delta t_{\text{eff}}(k, \Delta t) \frac{\partial \phi_k}{\partial \tau}, \tag{6}
\]

where the \(k\)-dependent effective time step is

\[
\Delta t_{\text{eff}}(k, \Delta t) \equiv \frac{\Delta t}{1 + \Delta t k^2[(a_1 - 1) + (1 - a_2)k^2]}, \tag{7}
\]

and \(\partial \phi_k/\partial \tau\) is the Fourier transform of \(\partial \phi/\partial \tau\) in Eq. (2) and is a function of \(\phi_k(t)\). As Eq. (7) reveals, the unconditionally stable algorithm has a mode-dependent effective time step \(\Delta t_{\text{eff}}(k, \Delta t)\). The optimal driving scheme for CH equation is an algorithmic time step \(\Delta t = A \tau^{2/3}\), where the prefactor \(A\) determines the accuracy [22,23].

On the other hand, the effective time-step for AC equation is

\[
\Delta t_{\text{eff}}(k, \Delta t) \equiv \frac{\Delta t}{1 + \Delta t[(a_1 - 1) + (1 - a_2)k^2]}, \tag{8}
\]

which indicates that
\[ \Delta t_{\text{eff}}(k, \Delta t) \leq \Delta t_{\text{eff}}(k, \infty) < \frac{1}{a_1 - 1}, \quad (9) \]

where \( a_1 - 1 > 0 \) and \( 1 - a_2 > 0 \) are used. We cannot obtain an accelerated algorithm in non-conserved systems since there is an upper bound for the effective time-step \( \Delta t_{\text{eff}}(k, \Delta t) \). In fact, the optimal driving scheme for AC equation is an algorithmic time step \( \Delta t = \infty \) [22].

3 Fourier space multi step error

In a computer simulation, assuming that we have updated the system \( m - 1 \) times, the algorithmic time is \( t_{m-1} \), and the field is \( \phi_k(t_{m-1}) \) in Fourier space. We next update the system using an algorithmic time step \( \Delta t_m \), and the field evolves according to Eq. (6):

\[ \phi_k(t_m) = \phi_k(t_{m-1}) + \Delta t_{\text{eff}}(k, \Delta t_m) \frac{\partial \phi_k}{\partial \tau}, \quad (10) \]

where \( t_m \equiv t_{m-1} + \Delta t_m \). To obtain the error of this unconditionally stable algorithm \( \Delta \phi_k \), we need to compare the field evolved by an unconditionally stable algorithm \( \phi_k(t) \) to the exact dynamics \( \phi_k(\tau) \) evolved by the same amount of energy [22,23]. The analytic time step \( \Delta \tau \) and the analytic time \( \tau \) can be determined by the energy evolution of each update [23]. At an analytic time \( \tau_{m-1} \), the system evolution after an analytic time step \( \Delta \tau_m \) is governed by the Taylor expansion:

\[ \phi_k(\tau_m) = \phi_k(\tau_{m-1}) + \sum_{n=1}^{\infty} \frac{\partial^n \phi_k}{\partial \tau^n} \Delta \tau_m^n \frac{1}{n!}, \quad (11) \]

where \( \tau_m \equiv \tau_{m-1} + \Delta \tau_m \). The Fourier space multi step error up to the \( m \)th update is

\[ \Delta \phi_k(m) \equiv \phi_k(t_m) - \phi_k(\tau_m). \quad (12) \]

Note that

\[ \Delta \phi_k(m) = \Delta \phi_k(m - 1) + \delta \phi_k(m), \quad (13) \]

where

\[ \delta \phi_k(m) = [\Delta t_{\text{eff}}(k, \Delta t_m) - \Delta \tau_m] \frac{\partial \phi_k}{\partial \tau} - \sum_{n=2}^{\infty} \frac{\partial^n \phi_k}{\partial \tau^n} \frac{\Delta \tau_m^n}{n!}. \quad (14) \]
We obtain that

$$\Delta \phi_k(m) = \sum_m \delta \phi_k(m) \approx \int \delta \phi_k dm,$$  \hfill (15)

where we use the integral to approximate the summation. Eq. (15) explains the numerical results that the single step error $\delta \phi_k(m)$ accumulates over time, which was observed in previous studies [22,23]. Note that as long as there is a distinction between the analytic time $\tau$ (time step $\Delta \tau$) and the algorithmic time $t$ (time step $\Delta t$), we can use Eq. (15) to calculate the Fourier space multi step error.

As an interesting application of the above result Eq. (15), we study the accuracy in the simplest Euler algorithm. The Euler algorithm has a mode-independent fixed time step $\Delta t_{Eu}$ to update the system, and $\Delta t_{eff}(k, \Delta t) = \Delta t_{Eu}$. In conserved systems, evolving from $\tau_0$ to $\tau_{\text{max}}$ with a fixed time step $\Delta t_{Eu} \approx \Delta \tau \sim d\tau/dm$ [23], we obtain the Fourier space multi step error as $kL \approx 1$:

$$\Delta \phi_k \sim -\frac{\tau_{\text{max}}}{\tau_0} \frac{\Delta t_{Eu}^2}{2} \tau^{-5/3} d\tau$$

$$= \frac{3\Delta t_{Eu}}{4} \left( \tau_{\text{max}}^{-2/3} - \tau_0^{-2/3} \right) \approx \frac{3\Delta t_{Eu}}{4} \tau_0^{-2/3},$$

(16)

where we ignore the higher order terms in the sum and $\partial^2 \phi_k / \partial \tau^2 \sim \tau^{-5/3}$ as $k \approx 1/L$ is used [23]. We can use this to determine the error in the scaled structure factor $g(kL) = \langle \phi_k \phi_{-k} \rangle / L^2$, where the angle brackets indicate an average over orientations and initial conditions. The absolute error is

$$\Delta g(kL) \approx \left| \frac{2\Delta \phi_k \phi_k}{L^2} \right| \sim \frac{\Delta t_{Eu} \tau_0^{-2/3}}{L},$$

(17)

where $\phi_k \sim L$ as $k \approx 1/L$ is used [23]. Since $L \sim \tau^{1/3} \to \infty$ at late times, the error $\Delta g(kL) \to 0$ at late times. This is why the Euler algorithm — or any fixed time step algorithm — is wastefully accurate.

4 Error in scaled structures

In this Section, we calculate the error in scaled structures due to the Fourier space multi step error determined in Section 3 with the optimal driving schemes discussed in Section 2.
4.1 Conserved systems

Using the formula discussed in Section 3, we obtain the Fourier space single step error with the optimal driving scheme \( \Delta t = A \tau^{2/3} \) [23]

\[
\delta \phi_k \sim \frac{L_0 C \sqrt{a_1 - 1}}{12 B^{1/3}} A^{3/2} \tau^{-1/6} k^{-1/2}
\]

(18)

where \( A, B \) and \( C \) are constants [23], and \( \partial \phi_k/\partial \tau \sim \tau^{-5/6} k^{-1/2} \) as \( k \gtrsim 1/L \) is used [see Appendix]. For a small \( A \), evolving from \( \tau_0 \) to \( \tau_{\text{max}} \) with time-step \( \Delta t = A \tau^{2/3} \approx \Delta \tau \sim d\tau/dm \), we obtain the Fourier space multi step error:

\[
\Delta \phi_k \sim \frac{L_0 C \sqrt{a_1 - 1}}{12 B^{1/3}} k^{-1/2} \int_{\tau_0}^{\tau_{\text{max}}} \frac{1}{A \tau^{2/3}} A^{3/2} \tau^{-1/6} d\tau
\]

\[
\approx \frac{L_0 C \sqrt{a_1 - 1}}{2 B^{1/3}} \sqrt{A} k^{-1/2} \tau_{\text{max}}^{-1/6}.
\]

(19)

We can use this result to determine the error in the scaled structure factor \( g(kL) = \langle \phi_k \phi_{-k} \rangle / L^2 \), where the angle brackets indicate an average over orientations and initial conditions. The absolute error is

\[
\Delta g(kL) \approx \left| \frac{2 \Delta \phi_k \phi_{-k}}{L^2} \right| \sim \frac{L_0 C \sqrt{a_1 - 1}}{B^{1/3}} \sqrt{A} \frac{1}{(kL)^2},
\]

(20)

where \( \phi_k \sim \tau_{\text{max}}^{-1/6} k^{-3/2} \) as \( k \gtrsim 1/L \) is used [see Appendix]. We can subsequently obtain the absolute error in the scaled derivative structure factor \( h(kL) = (kL)^2 g(kL) \):

\[
\Delta h(kL) = (kL)^2 \Delta g(kL) \sim \frac{L_0 C \sqrt{a_1 - 1}}{B^{1/3}} \sqrt{A}.
\]

(21)

To test Eq. (20), we measure \( S(k, t) = \langle \phi_k \phi_{-k} \rangle \), and obtain the time-independent scaling function \( \bar{S}(y) \equiv E^2 S(yE) \) using the energy density \( E \), where \( y \equiv k/E \). In Fig. 1 we plot the absolute difference between scaled structures obtained using an Euler algorithm and an unconditionally stable algorithm, \( \Delta \bar{S}(y) \) vs. \( y \). We find that \( \Delta \bar{S}(y) \sim y^{-2} \) as \( y \gtrsim 1 \), which implies \( \Delta g(x) \sim x^{-2} \) as \( x \gtrsim 1 \), where \( x \equiv kL \). We confirm the prediction in Eq. (20).
Fig. 1. The absolute difference between unconditionally stable and Euler updates, \( \Delta \tilde{S}(y) \) vs. \( y \equiv k/E \) for system size \( L_\infty = 512 \) at \( \tau = 1024 \). The Euler update used \( \Delta t_{Eu} = 0.03 \) and the unconditionally stable update used \( \Delta t = 0.01 \tau^{2/3} \). The plot shows that \( \Delta \tilde{S}(y) \sim y^{-2} \) as \( y \gtrsim 1 \), in agreement with Eq. (20).

4.2 Non-conserved systems

Using the formula discussed in Section 3, we obtain the Fourier space single step error with the maximal driving scheme \( \Delta t = \infty \) \[22\]

\[
\delta \phi_k \sim \left[ \frac{1}{a_1 - 1} - \Delta \tau_\infty \right] \tau^{-3/4} k^{-1/2},
\]

where \( \partial \phi_k / \partial \tau \sim \tau^{-3/4} k^{-1/2} \) as \( k \gtrsim 1/L \) is used [see Appendix]. Evolving from \( \tau_0 \) to \( \tau_{\text{max}} \) with time-step \( \Delta \tau_\infty \sim d\tau/dm \), we obtain the Fourier space multi-step error:

\[
\Delta \phi_k \sim k^{-1/2} \int_{\tau_0}^{\tau_{\text{max}}} \frac{1}{\Delta \tau_\infty} \left[ \frac{1}{a_1 - 1} - \Delta \tau_\infty \right] \tau^{-3/4} d\tau
\]

\[
\approx k^{-1/2} \tau_{\text{max}}^{-1/4} 4 \left[ \frac{\tilde{a}}{\xi \tan^{-1}(\tilde{a}/\xi)} - 1 \right],
\]

where

\[
\tilde{a} \equiv \sqrt{\frac{1 - a_2}{a_1 - 1}}.
\]

We then obtain the absolute error in scaled structure:
\[ \Delta g(kL) \approx \left| \frac{2\Delta \phi_k \phi_k}{L^2} \right| \sim \frac{8}{(kL)^2} \left[ \frac{\tilde{a}}{\xi \tan^{-1}(\tilde{a}/\xi)} - 1 \right], \tag{25} \]

where \( \phi_k \sim \tau_{\text{max}}^{1/4} k^{-3/2} \) as \( k \gtrsim 1/L \) is used [see Appendix]. We can subsequently obtain the absolute error in the scaled derivative structure factor \( h(kL) = (kL)^2 g(kL) \):

\[ \Delta h(kL) = (kL)^2 \Delta g(kL) \sim 8 \left[ \frac{\tilde{a}}{\xi \tan^{-1}(\tilde{a}/\xi)} - 1 \right] \tag{26} \]

This result indicates that the multi-step error in correlations increases with \( \tilde{a} \).

5 Error in analytic time step

In this Section, we calculate the error in analytic time step due to the error in scaled derivative structures (\( \Delta h \)) calculated in Section 4.

5.1 Conserved systems

CH systems are purely dissipative systems — the energy density \( E \) monotonically decreases with the analytic time \( \tau \) with the relation \( E \propto 1/L \propto \tau^{-1/3} \) [9]. We can calculate the analytic time in terms of the energy density \( E \):

\[ \tau = \frac{B_{CH}}{E^3}, \]

where the prefactor \( B_{CH} \) can be numerically determined by requiring \( \Delta \tau = \Delta t \) as \( \Delta t \to 0 \) in the late-time scaling regime since unconditionally stable algorithms are arbitrarily accurate as \( \Delta t \to 0 \). We can then calculate the analytic time step by differentiating \( \tau \) with respect to \( E \):

\[ \Delta \tau = \frac{-3B_{CH} \Delta E}{E^4} = -3\Delta E \tau^{4/3}/B_{CH}^{1/3}, \tag{27} \]

and \( \Delta E \) can be calculated by integrating from each Fourier mode:

\[ \Delta E = \int_0^{1/\xi} d^2k \frac{1}{(2\pi)^2} \left\langle \left( \frac{\delta F}{\delta \phi_k} \right) [\phi_k(t + \Delta t) - \phi_k(t)] \right\rangle = -\int_0^{1/\xi} d^2k \frac{1}{(2\pi k)^2} \Delta t_{\text{eff}}(k, \Delta t) T_k, \tag{28} \]
where the time derivative \( \partial \phi_k / \partial \tau = -k^2 \delta F / \delta \phi_k \) from Eq. (2), and \( \phi_k(t + \Delta t) - \phi_k(t) = \Delta \phi / \partial \phi_k / \partial \tau \) from Eq. (6) are used. The time-derivative correlation function \( T_k \) \cite{9,27,28} has a natural scaling form given by

\[
T_k \equiv \left\langle \frac{\partial \phi_k \partial \phi_{-k}}{\partial \tau \partial \tau} \right\rangle = \left( \frac{dL}{d\tau} \right)^2 h(kL) = \frac{L_0^2 h(kL)}{9 \tau^{4/3}}, \tag{29}
\]

where \( L = L_0 \tau^{1/3} \), \( h(x) \) is the 2D scaling function \cite{28}, and \( L_0 \) is a constant. Taking the error in scaled structures into account, \( h(x) \) takes the form \cite{28}

\[
h(x) = \frac{C_{CH}}{x} \pm \Delta h, \tag{30}
\]

as \( x \gtrsim 1 \), where \( C_{CH} \) is a constant and \( \Delta h \geq 0 \) is the absolute error in Eq. (21). The sign + or – will be determined later. Using the optimal driving scheme \( \Delta t = A \tau^{2/3} \) \cite{23}, we can solve for \( \Delta E \) in Eq. (28) and for the analytic time step \( \Delta \tau \) in Eq. (27). We have

\[
\Delta \tau = \frac{C_{CH} L_0^2 \Delta t}{6 \pi B_{CH}^{1/3}} \int_0^{L/\xi} \frac{dx}{x^2 [1 + (a_1 - 1)Ax^2/L_0^2]} \pm \frac{\Delta h L_0^2 \Delta t}{6 \pi B_{CH}^{2/3}} \int_{x_0}^{L/\xi} \frac{dx}{x [1 + (a_1 - 1)Ax^2/L_0^2]}, \tag{31}
\]

Solving the integral, we obtain

\[
\Delta \tau = \Delta t \left[ 1 - \left( \frac{L_0 C_{CH} \sqrt{a_1 - 1}}{12 B_{CH}^{1/3}} + d \right) \sqrt{A} + O(A) \right], \tag{32}
\]

where

\[
d \sim \frac{C L_0 \sqrt{a_1 - 1}}{12 \pi B_{CH}^{2/3}} \ln \left[ \frac{L_0^2}{(a_1 - 1)A} \right], \tag{33}
\]

and Eq. (21) is used. Note that we drop the + sign in Eq. (31) according to the requirement of \( \Delta \tau \leq \Delta t \) implied by Eq. (7). We have \( 1 - \Delta \tau / \Delta t \sim \sqrt{A} \), which is consistent with the previous results \cite{22,23}.
5.2 Non-conserved systems

Similar to the calculation in conserved systems, we can calculate the analytic time step by differentiating \( \tau \) with respect to \( E \):

\[
\Delta \tau = -\frac{2B_{AC} \Delta E}{E^3} = -\frac{2\Delta E \tau^{3/2}}{B_{AC}^{1/2}}. \tag{34}
\]

Integrating \( \Delta E \) from each Fourier mode, we have

\[
\Delta E \approx \frac{1}{2\xi} \int_0^{1/\xi} d^2k \left\langle \left( \frac{\delta F}{\delta \phi_k} \right) [\phi_k(t + \Delta t) - \phi_k(t)] \right\rangle
\]

\[
= -\frac{1}{2\xi} \int_0^{1/\xi} d^2k \Delta t_{eff}(k; \Delta t) T_k, \tag{35}
\]

where the time derivative \( \partial \phi_{-k}/\partial \tau = -\delta F/\delta \phi_k \) from Eq. (3), and \( \phi_k(t + \Delta t) - \phi_k(t) = \Delta t_{eff} \partial \phi_k/\partial \tau \) from Eq. (6) are used. The time-derivative correlation function \( T_k \) [9,27,28] has a natural scaling form of

\[
T_k = \left\langle \frac{\partial \phi_k \partial \phi_{-k}}{\partial \tau \partial \tau} \right\rangle = \left( \frac{dL}{d\tau} \right)^2 h(kL) = \frac{L_0^2 h(kL)}{4\tau}, \tag{36}
\]

where \( L = L_0 \tau^{1/2}, h(x) \) is the 2D scaling function [28], and \( L_0 \) is a constant. Taking the error in scaled structures into account, \( h(x) \) takes the form [28]

\[
h(x) = \frac{C_{AC}}{x} \pm \Delta h, \tag{37}
\]

as \( x \geq 1 \), where \( C_{AC} \) is a constant and \( \Delta h \geq 0 \) is the absolute error in Eq. (26). The sign + or – will be determined later. We can solve for \( \Delta E \) in Eq. (35) and for \( \Delta \tau \) from Eq. (34). We have

\[
\Delta \tau = \frac{C_{AC} \Delta t L_0}{4\pi B_{AC}^{1/2}} \tan^{-1} \left( \sqrt{\frac{\Delta t(1-a_2)}{1+\Delta t(a_1-1)}} \right)
\]

\[
\pm \frac{\Delta h L_0^2 \tau^{1/2}}{8\pi B_{AC}^{1/2}(1-a_2)} \ln \left( 1 + \frac{\Delta t(1-a_2)}{1+\Delta t(a_1-1)} \right). \tag{38}
\]

As \( \Delta t = \infty \), we obtain the maximal analytic time step:
\[ \Delta \tau_\infty = \frac{\xi \tan^{-1}(\tilde{a}/\xi)}{\sqrt{(a_1 - 1)(1 - a_2)}} - \frac{L_0^2 \ln(1 + \tilde{a}^2/\xi^2) \Delta h \tau^{1/2}}{8 \pi B_{AC}^{1/2}(1 - a_2)}, \tag{39} \]

where Eq. (26) is used. Note that we drop the + sign in Eq. (38) according to the requirement of \( \Delta \tau_\infty < 1/(a_1 - 1) \) implied by Eq. (9). Define

\[ \tilde{\Delta} \tau_\infty \equiv \Delta \tau_\infty \sqrt{(a_1 - 1)(1 - a_2)} = \xi \tan^{-1}\left(\frac{\tilde{a}}{\xi}\right) - f(\tilde{a})\tau^{1/2}, \tag{40} \]

where

\[ f(\tilde{a}) \sim \frac{L_0^2}{\pi B_{AC}^{1/2}} \left[ \frac{1}{\xi \tan^{-1}(\tilde{a}/\xi)} - \frac{1}{\tilde{a}} \right] \ln \left(1 + \frac{\tilde{a}^2}{\xi^2}\right). \tag{41} \]

Fig. 2. The discrepancy in the maximal analytic time step \( f(\tilde{a})\tau^{1/2} \) vs. the analytic time \( \tau \) in the scaling regime \((20 \leq \tau \leq 100)\) with \( \tilde{a} = 2 \) \((a_1 = 3 \text{ and } a_2 = -7)\) for system size \( L_\infty = 512. \) \( \xi \) is taken to be 0.92 for best fit by eye. The discrepancy shows a \( \tau^{1/2} \) behavior, as predicted in Eq. (40).

In a previous paper [22], we fitted the time-averaged \( \tilde{\Delta} \tau_\infty \) with \( \xi \tan^{-1}(\tilde{a}/\xi) \), and found that the fitting gets worse as \( \tilde{a} \) increases. This is consistent with the fact that \( f(\tilde{a}) \) monotonically increases with \( \tilde{a} \). In addition, for a chosen \( \tilde{a} \), in Fig. 2, we test the \( \tau \)-dependence of the discrepancy \( f(\tilde{a})\tau^{1/2} \) in the scaling regime and find excellent agreement.
6 Summary

We find it is interesting to compare the analytic time $\tau$ with the algorithmic time $t$. The analytic time $\tau$, determined by energy evolution, is a more fundamental quantity. The unconditionally stable update Eq. (6) is directly related to $\partial \phi_k / \partial \tau$, and all scaling analysis is in analytic time $\tau$. The algorithmic time step $\Delta t$, on the other hand, is a more practical quantity. It appears in the driving scheme and is used to express the Fourier space effective time step and to calculate the analytic time step. Our accuracy study on the scaled correlations $g(x)$ and $h(x)$ and subsequently on the analytic time step $\Delta \tau$ based on the error accumulation relation Eq. (15) were verified by numerical simulations. The analytic time step, the effective time step, the algorithmic time step, and the Fourier space multi step error are fundamental in understanding the error behavior in unconditionally stable algorithms for coarsening systems. The methodology can be readily generalized to study other systems. We hope to report that work in a subsequent paper.

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A Scaling of field derivatives in Fourier space

In order to explore the accuracy of unconditionally stable algorithms in Fourier space, it is necessary to know the scaling of field derivatives for all modes. The structure factor $S(k) = \langle |\phi_k|^2 \rangle = L^2 g(kL)$, where $g(kL) \sim (kL)^{-3}$ as $k \gtrsim 1/L$ [9]. Therefore we obtain

$$\phi_k \sim L^3 (kL)^{-3/2} = k^{-3/2} L^{-1/2}. \quad (A.1)$$

Previous studies [9,28] showed that $\partial \phi_k / \partial \tau = (dL/d\tau) \phi_k$ as $kL \gtrsim 1$. Then we obtain the time-derivative correlation function

$$T(k) = \langle |\partial \phi_k / \partial \tau|^2 \rangle = (dL/d\tau)^2 k^2 \langle |\phi_k|^2 \rangle = (dL/d\tau)^2 h_1(kL), \quad (A.2)$$

where the scaling function $h_1(kL) = k^2 L^2 g(kL) \sim (kL)^{-1} \sim L^{-1}$ as $k \gtrsim 1/L$. Subsequently we obtain
∂φ_k/∂τ \sim \frac{dL}{dτ}L^{-1/2}k^{-1/2}. \quad (A.3)

The generalization of higher order time-derivative correlations is

$$\langle |\partial^n \phi_k/\partial \tau^n|^2 \rangle \sim (dL/dτ)^2L^2\langle |\partial^{n-1} \phi_k/\partial \tau^{n-1}|^2 \rangle,$$

where “∼” indicates that generally the left hand side may not exactly equal to the right hand side. Applying this relation yields

$$\langle |\partial^n \phi_k/\partial \tau^n|^2 \rangle \sim (dL/dτ)^{2n}L^{2-2n}h_n(kL), \quad (A.4)$$

where \( h_n(kL) = k^2L^2h_{n-1}(kL) \sim (kL)^{2n-3} \) as \( k \gtrsim 1/L \). Therefore we have

$$\frac{\partial^n \phi_k}{\partial \tau^n} \sim \left( \frac{dL}{dτ} \right)^n L^{1-n}(kL)^{n-3/2},$$

$$\sim \begin{cases} 
\tau^{-2n/3-1/6}k^{n-3/2} & \text{conserved} \\
\tau^{-n/2-1/4}k^{n-3/2} & \text{non-conserved} 
\end{cases} \quad (A.5)$$

The above expression is valid for \( n \geq 0 \) for two dimensional scalar order parameter(s).

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