Controlling the accuracy of unconditionally stable algorithms in the Cahn-Hilliard equation

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Given an unconditionally stable algorithm for solving the Cahn-Hilliard equation, we present a general calculation for an analytic time step $\Delta\tau$ in terms of an algorithmic time step Δt. By studying the accumulative multistep error in Fourier space and controlling the error with arbitrary accuracy, we determine an improved driving scheme $\Delta t = At^{2/3}$ and confirm the numerical results observed in a previous study [Cheng and Rutenberg, Phys. Rev. E **72**, 055701(R) (2005)].

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The Cahn-Hilliard (CH) equation [1] models the phase separation that occurs during the quench of a conserved system from a high temperature isotropic phase into two distinct phases at low temperatures. The pattern of the two phase regions coarsens as the time τ increases, i.e., the length scale of these regions grows. At the later stages of this phase ordering process, the dynamics are dominated by a single length scale, the pattern domain size L, which increases with a power law in time τ, $L(\tau) \sim \tau^{1/3}$ [2]. This power-law growth implies that the motion of the domain walls becomes extremely slow at late times after a quench since a typical domain wall speed is $v \sim dL/d\tau \sim \tau^{-2/3}$, and a typical time scale for the interface to move a distance of order the interfacial width ξ is of order $\xi/v \sim \tau^{2/3}$.

Since there is no known analytic solution of the Cahn-Hilliard equation for random initial conditions, computational methods are necessary for investigation of such systems. The most straightforward approach is the Euler algorithm, which must employ a time step $\Delta t_{Eu} \sim (\Delta x)^4$ if stability is to be maintained, where Δx is the lattice spacing. Additionally, for Cahn-Hilliard systems, to resolve the interfacial profile, one has to use a lattice spacing $\Delta x < \xi$. The Euler fixed time step is suitable for update near the interface but wastefully accurate in the bulk at late times. This has been the main challenge of computer simulation of Cahn-Hilliard systems. The recently developed unconditionally stable algorithm [3–5] elegantly overcomes this difficulty. It allows a *mode-dependent* effective time step Δt_{eff}—a larger effective time step in the bulk as the domain size gets larger, while keeping the effective time step finite near the interfacial region [see Eq. (7)]. Since the unconditionally stable algorithm allows no constraints on time step, the main issue is ensuring the accuracy of the simulation. In a previous study [5], Cheng and Rutenberg numerically demonstrated that the error in correlations decreases monotonically as A decreases down to $A=0.001$, where A is a prefactor in the previous driving scheme $\Delta t = At_s^{2/3}$ and t_s is the structural time (see below for a precise definition). However, absence of computational power prevents us from exploring the error behavior for arbitrarily small A. For *arbitrary accuracy*, we need to rigorously prove that the error can be made *arbitrarily small*.

To achieve this goal, we must first distinguish two quantities generic to all numerical algorithms: *analytic time step* $\Delta\tau$ (*analytic time* τ) and *algorithmic time step* Δt (*algorithmic time* t). The former appears in the equation of motion and represents the time step (time) of the system evolution governed by the exact solution to the dynamical equations, while the latter appears in the finite difference scheme and represents the time step (time) of the system evolution by the computational algorithms. We now briefly review these two concepts and study why the distinction has been largely overlooked thus far.

In Euler algorithm, it is not necessary to distinguish the analytic time step and the algorithmic time step, since there is a threshold on the time step, and they are always approximately identical (see the analysis below). On the other hand, semi-implicit algorithms have no such threshold. An unconditionally stable algorithm, an extension of the semi-implicit method, allows for an arbitrarily large time step without encountering the numerical instabilities for suitably chosen parameters (as determined using a standard von Neumann stability analysis). Although this method has been in use for some time, there has been little analytic study about how to obtain maximal speedup while controlling the accuracy. Indeed, all the previous work known to us assumes no difference between the analytic time step and the algorithmic time step—one can only increase the time step modestly and assume the resulting error is small enough to be ignored.

In what follows, we perform a general calculation of the analytic time step $\Delta\tau$ in terms of the algorithmic time step Δt, and show how this relationship allows one to choose a driving scheme for arbitrary accuracy. Concomitantly, we demonstrate that the driving scheme can be improved to $\Delta t = At^{2/3}$. While the calculation presented is specifically applicable to the Cahn-Hilliard equation, much of our analysis is general and should guide subsequent studies of more complicated systems. For simplicity but without loss of generality, we restrict our analysis to two dimensions (2D).

The Cahn-Hilliard equation can be written as

$$\frac{\partial \phi}{\partial \tau} = \nabla^2 \frac{\delta F}{\delta \phi} = -\nabla^2(\phi + \nabla^2\phi - \phi^3), \tag{1}$$

where the free energy functional is

$$F \equiv \int d^2x \left[|\nabla \phi|^2 + \frac{(\phi^2-1)^2}{4} \right], \tag{2}$$

and $\phi(\mathbf{x},\tau)$ is a conserved scalar field (such as an appropriately scaled mass concentration) and the potential has a double-well structure that the equilibrium values are at $\phi = \pm 1$. To illustrate and distinguish the analytic time step from the algorithmic time step, we first study the exact dynamics of the Cahn-Hilliard systems Eq. (1) in Fourier space. At an analytic time τ, the system evolution after an analytic time step $\Delta\tau$ is governed by the Taylor expansion:

$$\phi_k(\tau+\Delta\tau) = \phi_k(\tau) + \sum_{n=1}^{\infty} \frac{\partial^n \phi_k}{\partial \tau^n} \frac{\Delta\tau^n}{n!}. \tag{3}$$

Using the results of the field derivatives in Fourier space Eq. (15), for a finite $\Delta\tau$, one finds that all $n \geq 2$ terms are negligible compared with the $n=1$ term. So we obtain the traditional Euler finite difference scheme

$$\phi_k(t+\Delta t_{Eu}) = \phi_k(t) + \Delta t_{Eu} \frac{\partial \phi_k}{\partial \tau}, \tag{4}$$

where $\partial\phi_k/\partial\tau$ is the Fourier transform of $\partial\phi/\partial\tau$ in Eq. (1) and is a function of $\phi_k(t)$. We see that the Euler algorithm uses first order finite differences to approximate the solution obtained by exact dynamics. On the other hand, an unconditionally stable algorithm is obtained by an appropriate semi-implicit discretization of Eq. (1) in algorithmic time:

$$\begin{aligned} &\phi_{t+\Delta t} + (1-a_1)\Delta t \nabla^2 \phi_{t+\Delta t} + (1-a_2)\Delta t \nabla^4 \phi_{t+\Delta t} \\ &\quad = \phi_t - \Delta t \nabla^2 (a_1 \phi_t + a_2 \nabla^2 \phi_t - \phi_t^3). \end{aligned} \tag{5}$$

Unconditionally stability is obtained for the choices $a_1 > 2$ and $a_2 < 0.5$ [4]. Here, $\phi_{t+\Delta t}$ represents the implicit terms and ϕ_t represents the explicit terms. We can solve Eq. (5) directly in Fourier space and obtain

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

where the k-dependent effective time step is

$$\Delta t_{eff}(k,\Delta t) \equiv \frac{\Delta t}{1 - \Delta t \lambda_{\mathbf{k}} [(a_1-1) + (a_2-1)\lambda_{\mathbf{k}}]}, \tag{7}$$

and $\lambda_{\mathbf{k}} = -k^2$ is the Fourier-transformed Laplacian. The Euler algorithm has a mode-independent fixed time step to update the system in Fourier space, but, as Eq. (7) reveals, the unconditionally stable algorithm has a mode-dependent effective time step $\Delta t_{eff}(k,\Delta t)$. A direct comparison of Eqs. (3) and (4) yields that the analytic time step $\Delta\tau$ is always a good approximation of the algorithmic time step Δt_{Eu} in Euler algorithm. However, for the unconditionally stable algorithm, a comparison of Eqs. (3) and (4) does not give a straightforward relation between $\Delta\tau$ and Δt, i.e., we do not know what $\Delta\tau$ corresponds to Δt. In what follows we explore the relationship between these two time steps in the CH equation, and the consequences this relationship has on the accuracy of the solution method. The steps of our procedure are shown in *italics*.

Calculate the analytic time and time step. We now calculate the analytic time step $\Delta\tau$ in terms of an algorithmic time step Δt. Cahn-Hilliard systems are purely dissipative systems — the energy density E monotonically decreases with the analytic time with the relation $E \propto \tau^{-1/3}$ [2]. Without such a relationship between a physical quantity and the analytic time, the analysis that is performed below cannot proceed, and thus progress in applying these methods to other models hinges on the physical insights needed to obtain such relationships (in this case the so-called "scaling hypothesis"). The analytic time is conveniently calculated in terms of the monotonically decaying energy density E: $\tau = B/E^3$, where the prefactor B can be numerically determined by requiring $\Delta\tau = \Delta t$ as $\Delta t \to 0$ in the late-time scaling regime since our unconditionally stable algorithm is arbitrarily accurate as $\Delta t \to 0$. Note that the calculation here is identical to the calculation of the *structural time* t_s in a previous study [5] since the structural time is just another representation of the *analytic time*.

We can calculate the analytic time step by differentiating τ with respect to E:

$$\Delta\tau = -3B\frac{\Delta E}{E^4} = -3\Delta E \frac{\tau^{4/3}}{B^{1/3}}, \tag{8}$$

and ΔE can be calculated by integrating ΔE from each Fourier mode:

$$\begin{aligned} \Delta E &\approx \int_0^{1/\xi} d^2k \frac{1}{(2\pi)^2} \left\langle \left(\frac{\delta F}{\delta \phi_k} \right) \Delta \phi_k \right\rangle \\ &= -\int_0^{1/\xi} d^2k \frac{1}{(2\pi k)^2} \Delta t_{eff}(k,\Delta t) T_k, \end{aligned} \tag{9}$$

where the time derivative $\partial\phi_{-k}/\partial\tau = -k^2 \delta F/\delta\phi_k$ from Eq. (1) and $\Delta\phi_k = \phi_k(t+\Delta t) - \phi_k(t) = \Delta t_{eff} \partial\phi_k/\partial\tau$ from Eq. (6) are used, and T_k is the time-derivative correlation function [2,6,7] and has a natural scaling form given by

$$T_k \equiv \left\langle \frac{\partial \phi_k}{\partial \tau} \frac{\partial \phi_{-k}}{\partial \tau} \right\rangle = \left(\frac{dL}{d\tau} \right)^2 h(kL) = \frac{L_0^2 h(kL)}{9\tau^{4/3}}, \tag{10}$$

where $L = L_0 \tau^{1/3}$, $h(x) = C/x$ is the 2D scaling function [7] as $x \gg 1$, and L_0 and C are constants. We can then solve for ΔE in Eq. (9) and for the analytic time step $\Delta\tau$:

$$\begin{aligned} \Delta\tau &= \frac{L_0^2 \Delta t}{6\pi B^{1/3}} \int_0^{\infty} \frac{dx}{x} \frac{h(x)}{1 + \Delta t (a_1-1) x^2/L^2} \\ &= \frac{C L_0^2 \Delta t}{6\pi B^{1/3}} \int_0^{\infty} \frac{dx}{x^2 (1 + D\ell^2 x^2)}, \end{aligned} \tag{11}$$

where $x = kL$, $D = (a_1-1)/L_0^2$, and $\ell = \sqrt{\Delta t/\tau^{2/3}}$. Solving the integral, we obtain that,

$$\Delta\tau = \Delta t [1 - \zeta \ell + O(\ell^2)], \tag{12}$$

where $\zeta = L_0 C \sqrt{a_1 - 1}/(12 B^{1/3})$. The above formula is the central result of this Brief Report, and implies that $\Delta\tau \leq \Delta t$ in general. We now explore how to use this result to obtain an accelerated algorithm.

Scaling of field derivatives in Fourier space. In order to explore the accuracy of accelerated algorithms in Fourier space, it is necessary to know the scaling of field derivatives both in the bulk (where $k \sim 1/L$) and near the interface (where $k \sim 1/\xi$). The structure factor $S(k)=\langle|\phi_k|^2\rangle=L^2 g(kL)$, where $g(kL)\sim 1$ as $k\sim 1/L$ and $g(kL)\sim(kL)^{-3}\sim L^{-3}$ as $k \sim 1/\xi$ [2]. Therefore we obtain

$$\phi_k \sim \begin{cases} \tau^{1/3} & \text{as } k \sim 1/L, \\ \tau^{-1/6} & \text{as } k \sim 1/\xi. \end{cases} \tag{13}$$

Previous studies [2,7] showed that $\partial\phi_k/\partial\tau=(dL/d\tau)k\phi_k$ as $kL\gg 1$, so we obtain the form for the time-derivative correlation function $T(k)=\langle|\partial\phi_k/\partial t|^2\rangle=(dL/d\tau)^2k^2\langle|\phi_k|^2\rangle=(dL/d\tau)^2h_1(kL)$, where the scaling function $h_1(kL)=k^2L^2g(kL)\sim 1$ as $k\sim 1/L$, and $h_1(kL)\sim(kL)^{-1}\sim L^{-1}$ as $k \sim 1/\xi$. Therefore we obtain

$$\frac{\partial\phi_k}{\partial\tau} \sim \begin{cases} \tau^{-2/3} & \text{as } k \sim 1/L, \\ \tau^{-5/6} & \text{as } k \sim 1/\xi. \end{cases} \tag{14}$$

The generalization of higher order time-derivative correlations is $\langle|\partial^n\phi_k/\partial\tau^n|^2\rangle\sim(dL/d\tau)^2k^2\langle|\partial^{n-1}\phi_k/\partial t^{n-1}|^2\rangle$, where "$\sim$" indicates that generally the left-hand side may not exactly be equal to the right-hand side. Applying this relation will yield $\langle|\partial^n\phi_k/\partial\tau^n|^2\rangle\sim(dL/d\tau)^{2n}L^{2-2n}h_n(kL)$, where $h_n(kL)=k^2L^2h_{n-1}(kL)\sim(kL)^{2n-3}\sim 1$ as $k\sim 1/L$, and $h_n(kL)\sim(kL)^{2n-3}\sim L^{2n-3}$ as $k\sim 1/\xi$. Therefore we have

$$\frac{\partial^n\phi_k}{\partial\tau^n} \sim \begin{cases} \tau^{-n+1/3} & \text{as } k \sim 1/L, \\ \tau^{-2n/3-1/6} & \text{as } k \sim 1/\xi. \end{cases} \tag{15}$$

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

Determine the driving scheme for arbitrary accuracy. Next, we determine the driving scheme for arbitrary accuracy in terms of the Fourier space error. Before we study the error, we must first distinguish the error in the bulk and the error near the interface. Equation (7) implies $\Delta t_{eff}\sim\tau^{2/3}$ as $k\sim 1/L$ and $\Delta t_{eff}\sim$const as $k\sim 1/\xi$, we obtain that the ratio of the single step field update with respect to the field $\Delta\phi_k/\phi_k\sim(\Delta t_{eff}\partial\phi_k/\partial\tau)/\phi_k$ is of order $O(\tau^{-1/3})$ as $k\sim 1/L$ and $O(\tau^{-2/3})$ as $k\sim 1/\xi$. Therefore the error near the interface is negligible compared with the error in the bulk, and we will only study the error of those modes where $k\sim 1/L$.

In Fourier space, we compare the field evolved by an unconditionally stable algorithm to the exact dynamics evolved by the *same amount of energy*. Using this criterion we obtain the Fourier space single step error

$$\begin{aligned} \Delta\phi_k^s &\equiv \phi_k(t+\Delta t)-\phi_k(t+\Delta\tau) \\ &= (\Delta t_{eff}-\Delta\tau)\frac{\partial\phi_k}{\partial\tau}-\sum_{n=2}^{\infty}\frac{\partial^n\phi_k}{\partial\tau^n}\frac{\Delta\tau^n}{n!} \\ &\sim \frac{1}{1+D\ell^2}[\zeta\ell^3+O(\ell^4)], \end{aligned} \tag{16}$$

where Eq. (12) and $\partial\phi_k/\partial\tau\sim\tau^{-2/3}$ as $k\sim 1/L$ are used. The values of ζ and D are finite. Assuming the algorithmic time step $\Delta t=A\tau^\beta$, then $\ell=\sqrt{A}\tau^{\beta/2-1/3}$. In order to obtain arbitrary accuracy for $\Delta\phi_k^s$ at arbitrarily large τ, we require that $\beta=2/3$ since $\beta>2/3$ will make the error uncontrolled (arbitrarily large) at arbitrarily large τ, and $\beta<2/3$ will make the algorithm wastefully accurate (error is always zero) at arbitrarily large τ. A is then selected so that a desired accuracy is obtained. Thus $\Delta t=A\tau^{2/3}$ and $\Delta\phi_k^s\sim O(\ell^3)\sim O(A^{3/2})$.

For small A, Eq. (12) implies that $\tau\approx t(1-\zeta\sqrt{A})$. Therefore we can express the algorithmic time step Δt in terms of algorithmic time t:

$$\Delta t = A(1-\zeta\sqrt{A})^{2/3}t^{2/3}\approx At^{2/3}. \tag{17}$$

Writing the driving algorithmic time step in terms of algorithmic time t instead of the analytic time τ has the computational advantage of avoiding an intermediate calculation of τ at each update, and thus makes the computational implementation more straightforward.

Accuracy in correlations. Lastly, we analytically confirm the numerical results in a previous study [5] that the error in structure factor scales as $\sqrt{A}$. The Fourier space single-step error Eq. (16) will at worst accumulate with each update. For a small A, evolving to τ with time step $\Delta t=At^{2/3}\approx A\tau^{2/3}\approx\Delta\tau\sim d\tau/dn$ requires a number of steps

$$n=\int dn\sim\int_0^\tau\frac{d\tau}{A\tau^{2/3}}=\frac{3\tau^{1/3}}{A}. \tag{18}$$

Therefore, at τ, we obtain the upper bound on the Fourier space multistep error:

$$\Delta\phi_k^m\sim\Delta\phi_k^s n\sim\frac{3A^{3/2}\tau^{1/3}}{A}\sim L\sqrt{A}. \tag{19}$$

We can use this to bound the error in the scaled structure factor $g(kL)=\langle|\phi_k|^2\rangle/L^2$. As was investigated in our previous numerical studies [5], this quantity is simply the magnitude of the difference between the structure factor obtained using an unconditionally stable algorithm with one using the exact dynamics at the *same energy*. As $k\sim 1/L$ (in the bulk), we obtain the maximum error:

$$\Delta g_{max}\approx\frac{2\Delta\phi_k^m\phi_k}{L^2}\sim\sqrt{A}, \tag{20}$$

where $\phi_k\sim L$ as $k\sim 1/L$ is used. Equation (20) is precisely the same as the results obtained in our previous, solely numerical, study [5]. Thus the error produced in the bulk dominates the total error, as it decays much slower than the error produced near the interface. This error accumulates over time and results in the error in the structure factor scaling as $\sqrt{A}$.

In summary, we have analyzed numerical methods for solving the Cahn-Hilliard equation. By explicitly distinguishing the analytic and algorithmic time steps, we have developed a relation between them and have obtained an optimal driving scheme $\Delta t=At^{2/3}$ under the requirement of arbitrary accuracy. With this driving scheme, we have proved that the upper bound of the multistep error in structure factor scales as $\sqrt{A}$, a result obtained by numerical methods in a previous study [5]. We note that the argument developed herein is

founded, ultimately, on the physical relationship between the domain size and the analytic time (based itself on the scaling hypothesis). For systems where such relationships exist, or can be derived, we expect that this analysis should generalize to other systems, such as the newly developed phase field crystal model [8,9]. We hope to report this work in a subsequent paper.

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