PHYSICAL REVIEW E **72**, 055701(R) (2005)

Maximally fast coarsening algorithms

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(Received 30 June 2005; published 16 November 2005)

We present maximally fast numerical algorithms for conserved coarsening systems that are stable and accurate with a growing natural time step $\Delta t = A t_s^{2/3}$. We compare the scaling structure obtained from our maximally fast conserved systems directly against the standard fixed time-step Euler algorithm, and find that the error scales as $\sqrt{A}$—so arbitrary accuracy can be achieved. For nonconserved systems, only effectively finite time steps are accessible for similar unconditionally stable algorithms.

DOI: 10.1103/PhysRevE.72.055701 PACS number(s): 05.10.−a, 02.60.Cb, 64.75.+g

Phase-ordering kinetics studies the evolution of structure after a quench from a disordered phase into an ordered phase. The later stages of most phase-ordering processes show universal scaling behavior described by a single growing length scale which increases as a power law in time, $L(t) \sim t^{\alpha}$, where $0 < \alpha \leqslant 1$ [1]. For the scalar order-parameter systems considered in this paper, $\alpha = 1/2$ and $1/3$ for nonconserved and conserved dynamics, respectively [1]. While these growth exponents and their universality can be understood in terms of interfacial motion leading to domain coarsening [2], the time-independent scaled structure that results is less well understood.

Computer simulation is an effective technique to systematically study these nonlinear, nonequilibrium coarsening systems. To maintain accuracy, the discretized dynamics must move interfaces *at most* a small fraction of the interfacial width, ξ, in a single time step Δt. This determines a maximal or natural time step of coarsening systems, $\Delta t_{\mathrm{nat}} \sim \xi/(dL/dt) \sim t^{1-\alpha}$, that grows in time. Unfortunately, common time discretizations are unstable for time steps above a fixed threshold determined by the lattice spacing Δx [3]. Any such fixed time-step algorithm is increasingly inefficient at late times compared to the natural time step. Various algorithms have been proposed to make simulations more efficient, including the cell-dynamical scheme [4] and Fourier spectral methods [5]. However, these approaches still require a fixed time step for numerical stability.

There is a newly developed class of unconditionally stable semi-implicit algorithms [6,7] that impose no stability constraints on the time step Δt, which then must be determined by accuracy considerations. Since we generally expect larger Δt to lead to larger errors, there is a tradeoff between speed and accuracy. This tradeoff is best resolved by picking growth rates for Δt that induce an error in the correlations that is approximately constant in magnitude throughout the scaling regime, where the magnitude can be chosen to be comparable to other systematic sources of error such as initial transients or finite-size effects. While an analysis of the errors of *single* growing time steps indicated that simple maximally fast algorithms have large local errors [7,8], this begs the question of how much those single-step errors accumulate in correlations at late times after the quench. Some types of single-step errors may be benign, allowing us to exceed the bounds given by the single-step analysis [7,8]. For example, small amounts of random thermal noise are irrelevant to the scaled structure [1].

In this paper, we compare the scaled correlations of unconditionally stable "Eyre" dynamics driven with a growing time step Δt to the correlations evolved with an explicit Euler update. The latter, while slow, provides an arbitrarily accurate reference at late times. For conserved Cahn–Hilliard dynamics [9], we obtain accurate correlations when the Eyre algorithms are driven at the natural or *maximal* time step,

$$\Delta t = \Delta t_{\mathrm{nat}} = A t_s^{2/3}, \tag{1}$$

for conserved dynamics. Here we introduce a "structural time" t_s to track the structural evolution of the system through the decreasing system energy [see Eq. (7) below]. We find that the correlation error scales as $\sqrt{A}$ for small A, and so can be made arbitrarily small. With a similar class of unconditionally stable algorithms for nonconserved dynamics [7], we find that only a fixed factor speedup is possible compared to the Euler algorithm as measured by the structural time t_s. We explain the accurate maximally fast conserved dynamics and the effectively slow nonconserved dynamics with a novel Fourier-space analysis of the accelerated dynamics.

Cahn–Hilliard dynamics of a conserved scalar field $\phi(\mathbf{r},t)$ are

$$\partial\phi/\partial t = \nabla^2 \delta F/\delta\phi = -\nabla^2(\phi + \nabla^2\phi - \phi^3), \tag{2}$$

where $F \equiv \int d^d x[(\nabla\phi)^2 + (\phi^2-1)^2/4]$ is the free energy in d spatial dimensions with a double-well potential corresponding to two distinct ordered phases at $\phi = \pm 1$. These dynamics can be semi-implicitly discretized in time by

$$\tilde{\phi}_{t+\Delta t} + (1-a_1)\Delta t\nabla^2\tilde{\phi}_{t+\Delta t} + (1-a_2)\Delta t\nabla^4\tilde{\phi}_{t+\Delta t} = \phi_t - \Delta t\nabla^2(a_1\phi_t + a_2\nabla^2\phi_t - \phi_t^3), \tag{3}$$

where the discretized dynamics are unconditionally stable for any $\Delta t > 0$ when $a_1 > 2$ and $a_2 < 0.5$ [7]. This equation im-

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plicitly defines the updated field, $\tilde{\phi}_{t+\Delta t}$, and can be directly solved in Fourier space to give an Euler-like update,

$$\tilde{\phi}_k(t+\Delta t) = \phi_k(t) + \Delta t_{eff}(k)\dot{\phi}_k, \tag{4}$$

where the k-dependent effective time step is

$$\Delta t_{eff}(k) \equiv \Delta t/(1-\Delta t K), \tag{5}$$

$\lambda_{\mathbf{k}}$ is the Fourier-transformed Laplacian ($\lambda_{\mathbf{k}}=-k^2$ in the continuum limit), and

$$K \equiv (a_1-1)\lambda_{\mathbf{k}} + (a_2-1)\lambda_{\mathbf{k}}^2. \tag{6}$$

We note that $K<0$ for unconditionally stable algorithms.

Our numerical work is done in two dimensions (2D), with systems of linear size $L_\infty=256$ (at least 200 samples) and $L_\infty=512$ (at least 20 samples). We use a lattice spacing $\Delta x=1$ and periodic boundary conditions. For Euler discretizations of the conserved dynamics, Eq. (3) with $a_1=a_2=1$, we use $\Delta t=0.03$, while for unconditionally stable discretizations we use $a_1=3$ and $a_2=0$.

The k-dependent effective time step in the Fourier dynamics leads us to investigate the *effective* evolution of the system after one algorithmic time step Δt. What time interval in the exact dynamics, Eq. (2), best compares with the result of the discretized dynamics, Eq. (3)? Since arbitrarily large Δt in Eq. (3) should lead to large discretization errors, the answer is not always Δt. We exploit the power-law decay of the free-energy density, $\epsilon \equiv F/V$, in the late-time scaling regime, $\epsilon \simeq (t/B)^{-\alpha} \sim 1/L$ [2], to introduce the "structural" time

$$t_s \equiv B\epsilon^{-1/\alpha}, \tag{7}$$

where $\alpha=1/3$ or $1/2$ for conserved or nonconserved coarsening, respectively. We numerically determine B such that the structural time step is identical to the algorithmic time step for small enough Δt such that discretization errors are negligible. We find (data not shown) $B=0.286$ for conserved dynamics and $B=0.105$ for nonconserved dynamics. In general we find that $\Delta t_s \leqslant \Delta t$ (see Figs. 2 and 3 below) for maximally fast time steps given by Eq. (1), with equality only as $A \to 0$. Structural time allows us to measure the effective speedup of our coarsening algorithms, is used to determine the time step, and also provides important insight into errors of the scaled structure.

We find that using the natural time step, Eq. (1), leads to accurate correlations in the scaling regime—as compared to systems evolved with a simple Euler time discretization. We measure $S(k,t)=\langle \phi_k \phi_{-k} \rangle$, where the angle brackets indicate an average over orientations and initial conditions. We obtain the scaling form using the energy density, ϵ, so that $\tilde{S}(x) \equiv \epsilon^2 S(x\epsilon)$ is a scaling function of $x \equiv k/\epsilon$. In Fig. 1 we plot $\tilde{S}(x)$ versus x to illustrate the excellent overlap between Euler (circles) and Eyre ("+") dynamics with $\Delta t = A t_s^{2/3}$ and $A=0.01$. To quantify the error we take the absolute value of the maximal value of the difference between the scaled structures (shown for general k/ϵ with triangles). We find that this maximum difference is approximately constant in magnitude throughout the scaling regime.

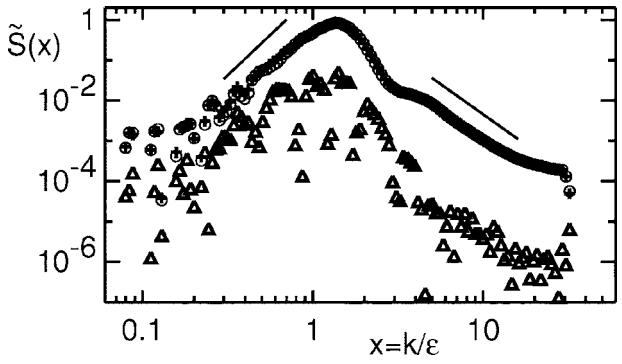

FIG. 1. The average scaled structure $\tilde{S}(x) \equiv \epsilon^2 S(x\epsilon)$ vs $x \equiv k/\epsilon$ for $L_\infty=512$ system at $t_s=1024$, with the Euler update (circles) with $\Delta t=0.03$ and the Eyre update ("+") with $\Delta t = A t_s^{2/3}$, where $A=0.01$. Triangles indicate the absolute difference between Eyre and Euler updates, $|\Delta \tilde{S}(x)|$.

We average this absolute error over the scaling regime, as determined by the scaling collapse of the scaled structure. We observe a small A-dependent difference between the Euler algorithm and the naturally driven Eyre algorithm, as shown in Fig. 2. By repeating the measurement for different system sizes, both $L_\infty=256$ (open circles, averaged over 4 times in $t_s \in [60,190]$) and $L_\infty=512$ (open squares, averaged over 9 times in $t_s \in [60,1500]$), we confirm that finite-size effects are not significant. We have enough independent Euler samples that no baseline errors due to residual stochastic effects are seen—the errors shown are the systematic error due to A. We observe an approximately $\sqrt{A}$ dependence on the average error. This implies that arbitrarily accurate measurements of the scaled structure can be made with maximally driven Eyre algorithms.

From the effective time step, Eq. (5), we can see qualitatively why the natural time step, Eq. (1), is accurate for conserved updates. Since Fourier modes $k \lesssim 1/L \sim t^{-1/3}$ correspond to the domain structure, then for the natural time step with very small A the effective timestep is only k-dependent deep in the Porod tail where $kL \gg 1$. However, the Porod tail

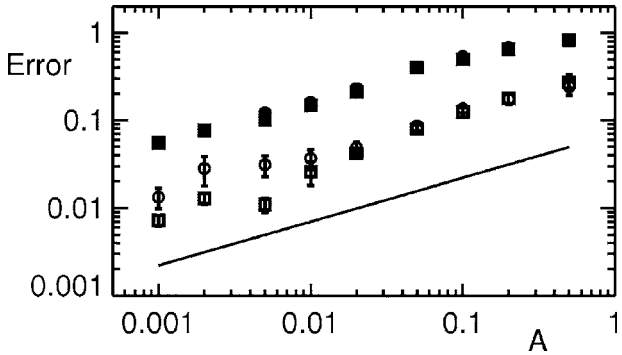

FIG. 2. The Eyre structural error vs A for Eyre algorithms driven at the natural time step $\Delta t = A t_s^{2/3}$. The error is the maximum absolute difference between the Eyre and the Euler correlations. Shown is data for $L_\infty=256$ (open squares) and $L_\infty=512$ (open circles). Also shown as filled symbols are the asymptotic values of $1-\Delta t_s/\Delta t$ for various A. Both errors exhibit $\sqrt{A}$ behavior, as discussed in the text.

[1] is simply the reflection of the amount of interface in the system at $kL \approx 1$. Systematic errors will arise as A gets larger and the k dependence of Δt_{eff} becomes more significant at $kL \approx 1$.

Previous real-space single-step error analysis [7] indicated that the natural time step would not be accurate for direct Eyre algorithms such as Eq. (3), because of growing local errors close to interfaces [8]. We have examined interfacial *profiles* of naturally driven algorithms, as probed by the $k \sim \xi^{-1}$ tail of the unscaled structure, and found quantitative agreement with the Euler algorithm (see large x data in Fig. 1). Single-step errors must then correspond to errors in the interfacial *motion*, which can be probed by considering the difference between the algorithmic time step Δt and the resulting structural time step Δt_s. We find that $\Delta t_s/\Delta t < 1$ in general, which indicates reduced interfacial motion. In Fig. 2 we show with filled symbols that $1-\Delta t_s/\Delta t$ scales as $\sqrt{A}$ for small A. We can recover this asymptotic result using an energy scaling argument [1,2] in general spatial dimension d.

From Eq. (7), with $\alpha = 1/3$ for conserved dynamics, we have $\epsilon = B^{1/3} t_s^{-1/3}$ so that

$$\Delta t_s = -3B^{-1/3} \Delta \epsilon t_s^{4/3}. \tag{8}$$

On the other hand, we can integrate the energy dissipated in one time step for each Fourier component [2],

$$\Delta \epsilon \simeq \int d^d k/(2\pi)^d \langle (\delta F/\delta \phi_k) \Delta \phi_k \rangle \tag{9}$$

$$= -\int d^d k/(2\pi)^d k^{-2} \Delta t_{eff}(k, \Delta t) T_k, \tag{10}$$

where the second line uses the time derivative $\dot{\phi}_{-k} = -k^2 \delta F/\delta \phi_k$ from Eq. (2), $\Delta \phi_k = \Delta t_{eff} \dot{\phi}_k$ from Eq. (4), and the time-derivative scaling function

$$T_k \equiv \langle \dot{\phi}_k \dot{\phi}_{-k} \rangle = \dot{L}^2 L^{d-2} h(kL), \tag{11}$$

where the scaling form is shown. T_k is expected to have a Porod-like $h(x) \sim x^{1-d}$ tail for $x \gg 1$ [2], and this has been observed in $d=2$ (data not shown). With these asymptotics and Δt_{eff} from Eq. (5), the $\Delta \epsilon$ integral converges and hence becomes time independent as the UV cutoff $O(L/\xi)$ becomes large. For $\Delta t = A t_s^{2/3}$ we obtain

$$\Delta t_s/\Delta t \propto \int_0^\infty dx x^{d-3} h(x)/(1 + A' x^2), \tag{12}$$

where $A' \equiv A(a_1 - 1)/L_0^2$ and $L = L_0 t_s^{1/3}$ in the scaling regime. For small A, the leading contribution is $O(\sqrt{A'})$ from the large x regime. Since $\Delta t_s/\Delta t = 1$ in the limit of $\Delta t \to 0$ when $A = 0^+$, we have

$$1 - \Delta t_s/\Delta t \propto \sqrt{A'} + O(A'). \tag{13}$$

This behavior is observed, as shown by the filled points in Fig. 2.

What is the connection, if any, between the time-step error $1-\Delta t_s/\Delta t$ and the structural error, both of which exhibit $\sqrt{A}$ dependence at small A for natural time steps? As discussed before, $1-\Delta t_s/\Delta t \sim \sqrt{A} > 0$ indicates an error of (reduced) interfacial motion. It is reasonable that this error shows up in the correlations at the same order, $O(\sqrt{A})$. It is interesting that this error accumulates into a constant contribution to the scaled correlations within the scaling regime.

We now consider nonconserved Allen–Cahn coarsening dynamics, which are governed by

$$\dot{\phi} = -\delta F/\delta \phi = \phi + \nabla^2 \phi - \phi^3. \tag{14}$$

These dynamics can be semi-implicitly discretized in time by

$$\tilde{\phi}_{t+\Delta t} + (a_1 - 1)\Delta t \tilde{\phi}_{t+\Delta t} + (a_2 - 1)\Delta t \nabla^2 \tilde{\phi}_{t+\Delta t} = \phi_t + \Delta t (a_1 \phi_t + a_2 \nabla^2 \phi_t - \phi_t^3), \tag{15}$$

where the discretized dynamics are unconditionally stable for any $\Delta t > 0$ when $a_1 > 2$ and $a_2 < 0.5$ [7]. In the same spirit as conserved dynamics, we obtain an effective time step

$$\Delta t_{eff}(k, \Delta t) = \Delta t/(1 - \Delta t N), \tag{16}$$

where $N \equiv (1-a_1) + (1-a_2)\lambda_{\mathbf{k}}$ and $N < 0$ for stable algorithms with $a_1 > 2$ and $a_2 < 0.5$ [7]. This directly implies that $\Delta t_{eff} \leqslant 1/(1-a_1)$ even when $\Delta t \to \infty$, so that this class of unconditionally stable nonconserved algorithms effectively cannot be accelerated. We confirm this by calculating and measuring Δt_s when $\Delta t = \infty$.

We adapt the development in Eqs. (8)–(12) for nonconserved dynamics. We have $\epsilon = B_{nc}^{1/2} t_s^{-1/2}$ so that

$$\Delta t_s = -2B_{nc}^{-1/2} \Delta \epsilon t_s^{3/2}. \tag{17}$$

Integrating the energy dissipated in one time step,

$$\Delta \epsilon \simeq -\int d^d k (2\pi)^{-d} \Delta t_{eff}(k, \Delta t) T_k, \tag{18}$$

where we use $\dot{\phi}_{-k} = -\delta F/\delta \phi_k$. Using Eq. (16) and Eq. (11) with $L = L_0 t_s^{1/2}$ and $\lambda_{\mathbf{k}} = -k^2$ we can solve for Δt_s when $\Delta t = \infty$,

$$\Delta t_s = \frac{L_0 L}{4\pi \sqrt{B_{nc}}} \int_0^{L/\xi} \frac{x^{d-1} h(x) dx}{(a_1 - 1)L^2 + x^2(1 - a_2)} \tag{19}$$

$$= \xi \frac{\tan^{-1}\left(\sqrt{\frac{1-a_2}{a_1 - 1}} \frac{1}{\xi} \right)}{\sqrt{(a_1 - 1)(1 - a_2)}}, \tag{20}$$

where we take the late-time $L \to \infty$ limit in the second line and have used $h_{nc}(x) \sim x^{1-d}$ for $x \gg 1$ [1,2], without which Δt_s is not time independent. The overall ξ factor on the second line comes from imposing $\Delta t_s = \Delta t$ for small Δt to determine B_{nc}, before the $\Delta t \to \infty$ limit is taken. We find a constant Δt_s that depends only on a_1 and a_2, as well as the inverse UV cutoff ξ. In Fig. 3, for $d=2$, we plot the measured asymptotic $\widetilde{\Delta t_s} \equiv \Delta t_s \sqrt{(a_1 - 1)(1 - a_2)}$ (averaged over the time-independent scaling regime with *variances* shown) versus $\tilde{a} \equiv \sqrt{(1-a_2)/(a_1 - 1)}$. We observe data collapse for a variety of a_1 and a_2, as suggested by Eq. (20). However, we only agree with the calculated functional form for small $\tilde{a}$—the solid line indicates best fit by eye with $\xi = 0.85$. The discrep-

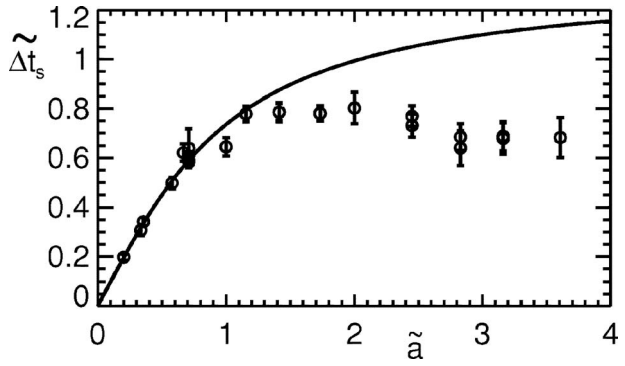

FIG. 3. For nonconserved update driven with $\Delta t=\infty$, we plot $\widetilde{\Delta t_s} \equiv \Delta t_s \sqrt{(a_1-1)(1-a_2)}$ vs $\tilde{a} \equiv \sqrt{(1-a_2)/(a_1-1)}$ showing the prediction (solid line with $\xi=0.85$) of Eq. (20).

ancy appears to be due to $\tilde{a}$ dependence of the time-derivative correlations (data not shown), indicating significant systematic errors when $\Delta t \to \infty$ despite the finite effective time step.

In summary, for conserved dynamics we obtain accurate scaled correlations for maximally fast algorithms with $\Delta t = A t_s^{2/3}$. The structural error behaves as $\sqrt{A}$ for small A. For these maximally fast algorithms the relative speedup with respect to a fixed time step is of the order $(L_\infty/\Delta x)^d$, where $L_\infty/\Delta x$ is the discretized linear system size. Maximally fast algorithms provide the most efficient means to reach the scaling limit for large systems.

Surprisingly, a similar class of algorithms does not lead to acceleration of nonconserved dynamics. Only a constant time step is observed, as measured by the structural time, even when the unconditionally stable algorithm is driven with $\Delta t \to \infty$. To explain these novel results, we have introduced the effective or structural time step Δt_s, which is calibrated to the decreasing energy of the system in the scaling regime when $\epsilon \sim 1/t^\alpha$. These results are consistent with previous real-space single-step error analysis [7] away from interfacial regions. With a Fourier-space analysis of the effective dynamics, we have shown that the large local errors found in a single-step real-space analysis of the dynamics [7] correspond to errors in domain-wall motion that accumulate into finite and controllable errors in the scaled correlations.

We expect that these unconditionally stable semi-implicit algorithms find a broader application. In the systems investigated so far, the regime of unconditional stability coincides with the easily determined regime of linear stability. For coarsening systems that exhibit a growing natural time step, large accelerations are possible with growing Δt. While the nonconserved dynamics cautions us that effective acceleration is not always achievable, it also illustrates the diagnostic value of the effective structural time step Δt_s. Indeed, $1 - \Delta t_s/\Delta t$ appears to provide a good proxy for systematic structural errors in the scaling regime.

We thank the Natural Science and Engineering Research Council of Canada and the Canadian Foundation for Innovation for support. We thank Ben Vollmayr-Lee for valuable ongoing discussions.

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