Maximally-fast coarsening algorithms

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

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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 in simple systems 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 $0 < \alpha \leq 1$ [1]. For the scalar order-parameter systems considered in this paper, $\alpha = 1/2$ and $1/3$ for non-conserved 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 result is less well understood.

Computer simulation is an effective technique to systematically study these non-linear non-equilibrium coarsening systems. To maintain accuracy, the discretized dynamics must move interfaces at most a small fraction of the interfacial width, $\xi$, in a single timestep $\Delta t$. This determines a maximal or natural timestep of coarsening, $\Delta t_{nat} \sim \xi/(dL/dt) \sim t^{1-\alpha}$, that grows in time. Unfortunately common time-discretizations are unstable for timesteps above a fixed threshold determined by the lattice spacing $\Delta x$ [3]. Any such fixed timestep algorithm is increasingly inefficient at late times compared to the natural timestep. Various algorithms have been proposed to make simulations more efficient, including the cell-dynamical-scheme [2] and Fourier spectral methods [2]. However, these approaches still require a fixed time-step for numerical stability.

There is a newly developed class of unconditionally stable semi-implicit algorithms [1,3] that impose no stability constraints on the timestep $\Delta t$, which is then determined by accuracy considerations. Since we generally expect larger $\Delta t$ to lead to larger errors, there is a trade-off between speed and accuracy. This tradeoff is best resolved by picking growth rates for $\Delta t$ 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 less than other systematic sources of error such as initial transients or finite-size effects. While errors of single growing timesteps can be small [5], this begs the question of how much those single-step errors accumulate in correlations at late times after the quench. For example, we might expect that some types of single-step errors would be benign, given the irrelevance of small amounts of random thermal noise to the scaled structure [1]. Nevertheless, we would expect timesteps growing faster than $\Delta t_{nat}$ to lead to unacceptable levels of error.

In this paper, we compare the scaled correlations of unconditionally stable “Eyre” dynamics driven with a growing timestep $\Delta t$ with 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 [4], we find that the maximal difference of the scaled structure has a constant magnitude in the scaling regime when the Eyre algorithms are driven at the natural or maximal timestep

$$\Delta t = At_s^{2/3},$$

for conserved dynamics. Here $t_s$ is a natural “structural time” determined by the decreasing system energy (see Eq. [4] below). We find that this correlation error scales as $\sqrt{A}$ for small $A$, and so can be made arbitrary small while retaining a maximally fast conserved coarsening algorithm which corresponds to moving interfaces a finite fraction of the interfacial width in every timestep. With a similar class of unconditionally stable algorithms for non-conserved dynamics [3], we find that only a fixed factor speedup is possible compared to the Euler algorithm as measured by the structural time $t_s$. With a Fourier-space analysis of the dynamics, we explain how the natural timestep can accurately be used in conserved coarsening while only a fixed timestep is possible for non-conserved coarsening.

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

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

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

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

where the discretized dynamics are unconditionally stable for any $\Delta t > 0$ when $a_1 > 2$ and $a_2 < 0.5$. This equation implicitly defines the updated field, $\phi_{t+\Delta t}$, and can be directly solved in Fourier space to give an Euler-like update

$$\tilde{\phi}_k(t + \Delta t) = \phi_k(t) + \Delta t e_{ff}(k) \phi_k$$

where the $k$-dependent effective timestep is

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

where $\lambda_k$ is the Fourier-transformed Laplacian ($\lambda_k = -k^2$ in the continuum limit), and

$$K \equiv (a_1 - 1) \lambda_k + (a_2 - 1) \lambda_k^2.$$  

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 timestep in Eq. 4 led us to investigate the actual timestep taken for a given algorithmic timestep $\Delta t$. To do this we exploit the power-law decay of the free-energy density, $\epsilon$, 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 $\tilde{S}(x)$ vs. $x$ to illustrate the excellent overlap between Euler (circles) and Eyre (“$$”) dynamics with $\Delta t = At^{2/3}$ 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 $k/\epsilon$ with triangles). We find that this maximum difference is approximately constant in magnitude throughout the scaling regime.

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 $t_s \in [60, 1900]$), 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 $1/A$ 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 timestep, Eq. 5, we can see qualitatively why the natural timestep, Eq. 11, 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 timestep with very small $A$ the effective timestep is only $k$-dependent deep in the Porod tail where $kL \gg 1$. However, the Porod tail 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 $\Delta t_{eff}$ becomes more significant at $kL \approx 1$.

Previous real-space single-step error analysis\(^5\) indicated that the natural timestep would not be accurate for direct Eyre algorithms like Eq. (1) because of growing errors close to interfaces\(^8\). We have examined interface profiles of naturally driven algorithms, as probed by the $k \sim \xi^{-1}$ tail of the unscaled structure, and found quantitative agreement with 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 timestep $\Delta t$ and the resulting structural timestep $\Delta t_s$. 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 recover this asymptotic result using an energy-scaling argument\(^1\) in general spatial dimension $d$.

From Eq. (4), with $\alpha = 1/3$ for conserved dynamics, we have $\epsilon = B^{1/3}s^{-1/3}$ so that

$$\Delta t_s = -3B^{-1/3}\Delta t_{eff}^{1/3}. \quad (8)$$

On the other hand we can integrate the energy dissipated in one timestep for each Fourier component\(^2\),

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

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

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

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

where the scaling form is shown. $T_k$ is expected to have a Porod-like $h(x) \sim x^{-d}$ tail for $x \gg 1$\(^2\) and this has been observed in $d = 2$\(^10\). With these asymptotics and $\Delta t_{eff}$ from Eq. (3), the $\Delta t$ integral converges and hence becomes time-independent as the UV cutoff $O(L/\xi)$ becomes large. For $\Delta t = At_s^{2/3}$ we obtain

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

where $A' \equiv A(a_1 - 1)/L_0^2$ and $L = L_0^{1/3}$ 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 $\Delta t \rightarrow 0$ when $A = 0^+$, we have

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

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

What is the connection, if any, between the timestep error $1 - \Delta t_s/\Delta t$ and the structural error, both of which exhibit $\sqrt{A}$ dependence at small $A$ for natural timesteps? 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 non-conserved Allen-Cahn coarsening dynamics, which are governed by

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

These dynamics can be semi-implicitly discretized in time by

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

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 timestep

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

where $N \equiv (1 - a_1) + (1 - a_2)\lambda_k$ and $N < 0$ for stable algorithms with $a_1 > 2$ and $a_2 < 0.5$\(^7\). This directly implies that $\Delta t_{eff} \leq 1/(1 - a_1)$ even when $\Delta t \rightarrow \infty$, so that this class of unconditionally stable non-conserved algorithms effectively cannot be accelerated. We confirm this by calculating and measuring $\Delta t_s$ when $\Delta t = \infty$.

We adapt the development in Eq. (3) - (12) for non-conserved dynamics. We have $\epsilon = B_{nc}^{1/2}t_s^{-1/2}$ so that

$$\Delta t_s = -2B_{nc}^{1/2} \Delta t_{eff}^{1/2} \quad (17)$$
Integrating the energy dissipated in one timestep,
\[ \Delta \epsilon \simeq - \int d^d k (2\pi)^{-d} \Delta t_{\text{eff}}(k, \Delta t) T_k \]
where we use \( \dot{\phi}_{-k} = -\delta F/\delta \phi_k \). Using Eq. (16) and Eq. (11) with \( L = L_0 t_1^{1/2} \) and \( \lambda_k = k^2 \) we can solve for \( \Delta t_s \) when \( \Delta t \to \infty \):
\[ \Delta t_s = \frac{L_0 L}{4\pi B_{nc}} \int_0^{L/\xi} \frac{x^{d-1} h(x) dx}{(a_1 - 1) L^2 + x^2 (1 - a_2)} \]
\[ = \frac{\tan^{-1} \left( \sqrt{\frac{1 - a_2}{a_1 - 1}} \frac{1}{\xi} \right)}{\sqrt{(a_1 - 1)(1 - a_2)}}. \]
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 \( x \gg 1 \), without which \( \Delta t_s \) is not time-independent. The overall \( \xi \) factor on the second line comes from imposing \( \Delta t_s = \Delta t \) for small \( \Delta t \) to determine \( B_{nc} \), before the \( \Delta t \to \infty \) limit is taken. We find a constant \( \Delta t_s \) that depends only on \( a_1 \) and \( a_2 \), as well as the inverse UV cutoff \( \xi \). In Fig. 3 for \( d = 2 \), we plot the measured asymptotic \( \Delta t_s \equiv \Delta t_s \sqrt{(a_1 - 1)(1 - a_2)} \) (averaged over the time-independent scaling regime with variances shown) vs. \( \tilde{a} \equiv \sqrt{(1 - a_2)/(a_1 - 1)} \). 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 discrepancy 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 timestep.

In summary, we have shown that 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 \( A \). These results are consistent with previous real-space single-step error-analysis away from interfacial regions. For these maximally fast algorithms the relative speedup with respect to a fixed timestep 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 non-conserved dynamics. Only a constant time-step is observed, as measured by the structural time, even when the unconditionally stable algorithm is driven with \( \Delta t \to \infty \).

We expect that these unconditionally-stable semi-implicit algorithms find 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 timestep, large accelerations are possible with growing \( \Delta t \). While the non-conserved dynamics cautious us that effective acceleration is not always produced, it also illustrates the diagnostic value of the ratio \( \Delta t_s/\Delta t \). Indeed, \( 1 - \Delta t_s/\Delta t \) appears to provide a good proxy for systematic structural errors in the scaling regime.

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