Abstract

We demonstrate and explain that conventional finite difference schemes for direct numerical integration do not approximate the continuum Kardar-Parisi-Zhang (KPZ) equation due to microscopic roughness. The effective diffusion coefficient is found to be inconsistent with the nominal one. We propose a novel discretization in 1+1 dimensions which does not suffer from this deficiency and elucidates the reliability and limitations of direct integration approaches.

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The Kardar-Parisi-Zhang (KPZ) equation has been very successful in describing a class of dynamical self-affine interfaces \([1]\). Numerous simulations on discrete models for vapor deposition, bacterial colony growth, directed polymers, etc. show agreements with KPZ predictions. Being the simplest nonlinear stochastic evolution equation for interfaces, the KPZ equation is believed to be relevant to a large diversity of phenomena although experimental verifications has been controversial \([1]\). Many numerical investigations on the subject have concentrated on discrete models. This work focuses on another important approach, namely, direct numerical integration of the KPZ equation. Amar and Family first conducted such large-scale integrations \([2]\). They found scaling exponents of the resulting interfaces in agreement with those from discrete models. This conclusion is supported subsequently by more accurate works indicating the validity of the KPZ approach \([3,4]\).

However, it has been observed that the discretized equations in the numerical integration of the KPZ equation admit peculiar properties not fully compatible with their continuum counterparts \([3,4]\). By applying Lam and Sander’s inverse method \([7]\), we will give a quantitative demonstration and theoretical explanation of an abnormal behavior of the diffusion coefficient. We propose a novel discretization for the numerical integration of KPZ interfaces in 1+1 dimensions. Our discrete equations behaves in a much more predictable way as proved by exact solution of its steady state properties. The results should clarify the reliability and limitations of conventional numerical integration techniques on the KPZ equation. In addition, conventional direct numerical integration schemes for the KPZ equation are inefficient and numerically rather unstable at high nonlinearity \([2,4]\). We will give a quantitative evaluation of this instability. In contrast, the new discrete equations can be integrated substantially more efficiently with much improved stability.

The KPZ equation gives the local rate of growth of the coarse-grained height profile \(h(x, t)\) of an interface at substrate position \(x\) and time \(t\) \([1]\):

\[
\frac{\partial h}{\partial t} = c + \nu \nabla^2 h + \frac{\lambda}{2} (\nabla h)^2 + \eta(x, t),
\]

where \(c\), \(\nu\) and \(\lambda\) are the average growth rate, the diffusion coefficient and the nonlinear
parameter respectively. There is an implicit lower wavelength cutoff below which \( h \) is smooth. The noise \( \eta \) has a Gaussian distribution and mean 0 and a correlator \( \langle \eta(x, t)\eta(x', t') \rangle = 2D\delta(x - x')\delta(t - t') \). Most previous works on the numerical integration of the KPZ equation adopt the finite difference and Euler’s method with the following equation [2–4]:

\[
h_{i}^{n+1} = h_{i}^{n} + \Delta t \left[ \nu_{0} (h_{i+1}^{n} + h_{i-1}^{n} - 2h_{i}^{n}) + \left( \lambda_{0}/8 \right) (h_{i+1}^{n} - h_{i-1}^{n})^{2} \right] + \sqrt{2D_{0}\Delta t} \xi_{i}^{n},
\]

where \( h_{i}^{n} \) approximates \( h(i\Delta x, n\Delta t) \) with periodic boundary conditions and every \( \xi_{i}^{n} \) is an independent Gaussian variable with zero mean and unit variance. The subscripted parameters \( \nu_{0}, \lambda_{0} \) and \( D_{0} \) are nominal values used in the iteration to be distinguished from the continuum values in the KPZ description in Eq. (1). Following previous works [2,3,1], the spatial step size \( \Delta x \) is taken to be 1. Other choices will be discussed later. The implicit lower wavelength cutoff here is effectively 1 due to the spatial discretization. The temporal step size \( \Delta t \) is taken to be small enough so that decreasing its value further will not alter the results.

In fact, it can be verified easily that as long as it is numerically stable, \( \Delta t \) need not be small before the KPZ scaling exponents can be computed accurately. This is because the discrete equation with finite \( \Delta t \) is by itself in the KPZ universality class similar to many discrete models due to symmetry considerations. The reason for taking a small \( \Delta t \) is to allow the discrete equation to approximate the continuum KPZ equation. However, we suggest that finite differencing is not a good approximation because of microscopic roughness, although this does not alter the scaling exponents due to universality.

Naively assuming that \( h(x, t) \) is smooth at the lattice level, the error of discretization is \( O(\Delta x^{2}) \). Figure 1 shows the details of an interface generated using Eq. (2). In all numerical simulations in this letter, we put \( \nu_{0} = D_{0} = 1 \). Other choices can be recast into this form by rescaling the height and the time scales [2]. Here, we have taken \( \lambda_{0} = 3 \) corresponding to medium nonlinearity and \( \Delta t = 0.01 \) and a smaller \( \Delta t \) gives similar results. Existence of microscopic roughness is evident and hence errors due to the spatial discretization are
uncontrolled. Therefore, there is no apriori reason why Eq. (2) should approximate Eq. (1) unless there exist special reasons such as conservation laws as in the linear $\lambda_0 = 0$ case.

We apply the inverse method [7] to examine interfaces generated using Eq. (2) with the same parameters $\nu_0 = D_0 = 1$, $\lambda_0 = 3$ and $\Delta t = 0.01$ on a lattice of size $L = 32768$. This approach computes all the parameters in the corresponding continuum KPZ description in Eq. (1). The method extracts the continuum parameters by requiring them, when plugged into Eq. (1), to give the best prediction on the evolution of a surface coarse-grained up to length $l$ during a period $\tau$. Hence $l$ and $\tau$ are respectively the spatial and temporal resolutions of observation [7]. Figure 2 shows the results. Continuum parameters are extracted at large $l$ where finite size effects are insignificant. We obtain the unrenormalized parameter $\lambda \simeq 3.04$. The values $\nu$ and $D$ are renormalized in the same way due to a fluctuation dissipation theorem [8] and we have $D/\nu \simeq 0.88$ for all $\tau$. At large $l$, $\tau$ controls the extent of renormalization since it dictates how short the wavelength of the modes should be to evolve fast enough to contribute to renormalization [7]. At small $\tau$ corresponding to the short time limit in which no renormalization has taken place, we obtain the unrenormalized parameters $D \simeq 1.007$ and $\nu \simeq 1.14$. We thus have $\lambda \simeq \lambda_0$ and $D \simeq D_0$ consistent with the validity of the finite difference approximation. Unfortunately, it is clear that $\nu \neq \nu_0$. We check the result by calculating the ratio $D/\nu$ independently from the correlation function [10]:

$$C(r) = <[h(x+r,t) - h(x,t)]^2> = (D/\nu)r,$$

where the last equality is true for large $r$. We obtain $D/\nu \simeq 0.86$ in reasonable agreement with the inverse method estimate. We have also repeated the measurements for a much smaller $\Delta t = 0.00125$. The ratio $D/\nu$ estimated from both the inverse method and the correlation function is indistinguishable from the previous results within our statistical error which is less than $\pm 0.02$. Our estimates of $D/\nu$ in the range 0.86 to 0.88 are distinctly different from $D_0/\nu_0 = 1$. We conclude that the discrete equation (2) is in the KPZ universality class and is closely related to but does not approximate the continuum KPZ equation (1). This point will be explained later.
It should be noted that decreasing $\Delta x$ is not a valid way to improve the accuracy of the finite difference scheme but is simply equivalent to diminishing the nonlinear parameter $\lambda$. This is because any value of $\Delta x$ can be rescaled back to 1 by the transformation $x \to (\Delta x)^{-1}x$, $t \to (\Delta x)^{-2}t$, $h \to (\Delta x)^{-1/2}h$ which leaves Eq. (1) invariant except that $\lambda$ is now replaced by $(\Delta x)\lambda$. In general, maintaining sufficient nonlinearity of the system is essential to exhibit any relevant properties of the KPZ class. It is most convenient to fix $\Delta x = 1$ and adjust the nonlinearity using $\lambda$ as in Ref. [2,3,1], although tuning the nonlinearity with $\Delta x$ has also been done [4].

To further understand the anomaly, it is instructive to study the following novel discretization which does give a correct diffusion coefficient:

$$\frac{dh_i}{dt} = \nu_0 \Gamma_i + \frac{\lambda_0}{2} \Psi_i + \eta_i(t),$$

for $i = 1$ to $L$ with periodic boundary conditions, where

$$\Gamma_i = h_{i+1} + h_{i-1} - 2h_i$$

$$\Psi_i = (1/3)[(h_{i+1} - h_i)^2 + (h_{i+1} - h_i)(h_i - h_{i-1})$$

$$+ (h_i - h_{i-1})^2].$$

The noise $\eta_i(t)$ has a Gaussian distribution and $< \eta_i(t)\eta_j(t') > = 2D_0 \delta_{ij} \delta(t-t')$. Both Eqs. (4) and (1) could be equally valid $O(\Delta x^2)$ spatial discretizations of Eq. (1) if the interface were smooth. However, neither are necessarily a good finite difference approximation of Eq. (1) due to the microscopic roughness.

The steady state properties of the new equations admit elegant exact solutions. Let $P[h,t]$ be the probability distribution of the discrete interface $\{h_i\}_{i=1}^L$ at time $t$. It obeys the Fokker-Planck equation [1]:

$$\frac{\partial P}{\partial t} = -\sum_{i=1}^L \frac{\partial}{\partial h_i} \left[ \left( \nu_0 \Gamma_i + \frac{\lambda_0}{2} \Psi_i \right) P \right] + D_0 \sum_{i=1}^L \frac{\partial^2 P}{\partial h_i^2}$$

which has the exact steady state solution:

$$P[h] = \exp \left[ -\frac{\nu_0}{2D_0} \sum_i (h_{i+1} - h_i)^2 \right].$$
The existence of this exact solution results from the vanishing of the $\lambda_0$ term on the RHS of Eq. (7) when Eq. (8) is applied, in complete analogy with the continuum case [1]. The specific form of $\Psi_i$ in Eq. (4) is specifically chosen to allow for the cancelation and this property is not shared by other discretizations in general.

We now calculate the associated continuum parameters in the KPZ description of Eq. (4). Assuming a large lattice, it follows from Eq. (8) that the correlation function is $C(r) = (D_0/\nu_0)r$. Comparing with the continuum result in Eq. (3), we obtain $D/\nu = D_0/\nu_0$. At the short time limit, the noise terms dominate in both Eqs. (4) and (1) and it is easy to see that the continuum short time noise parameter is $D = D_0$. Hence, the short time continuum diffusion coefficient is $\nu = \nu_0$. To calculate $\lambda$, we consider a screw boundary condition so that the interface has an average slope $u$. The steady state probability distribution now becomes $P[h] = \exp \left[ -\left( \nu_0/2D_0 \right) \sum_i (h_{i+1} - h_i - u)^2 \right]$. It is then easy to show that the average growth velocity is $v(u) = \langle \partial h_i/\partial t \rangle = \lambda_0/3 + \lambda_0 u^2/2$. The continuum nonlinear parameter can be calculated from $\lambda = v''_\infty(0)$ [10] and we get $\lambda = \lambda_0$. The average growth velocity is $c = v(0) = \lambda_0/3$. Therefore, all three continuum parameters $\nu$, $\lambda$ and $D$ are exactly the respective nominal values $\nu_0$, $\lambda_0$ and $D_0$ in the new discretization. These results are confirmed numerically using both the inverse method and measurements of correlation functions.

To gain further insights, we calculate the short time value of $\nu$ directly by a novel analytical application of the inverse method. When calculating the continuum parameters $c$, $\nu$ and $\lambda$ disregarding any higher order terms, the inverse method reduces the problem to the solution of a matrix equation [7]. Due to an up-down symmetry of the interfaces at long length scales [8], the matrix is block diagonal at large spatial resolution $l$ and the expression for $\nu$ is simplified to

$$\nu = \frac{\langle (\partial h/\partial t)_{c} (\partial^2 h/\partial x^2)_{c} \rangle_c}{\langle (\partial^2 h/\partial x^2)_{c}^2 \rangle_c}$$

(9)

where the subscript $c$ denotes coarse graining to length scale $l$ before evaluation at a given lattice point $i$. The operation $\partial/\partial x$ is usually carried out in the Fourier space. The growth
rate \((\partial h/\partial t)_c\) is contributed by \(\Gamma\) and \(\Psi\) in Eqs. (4)-(6) while effects of the noise vanish after averaging. Now the steady state distribution \(P[h]\) in Eq. (8) is invariant under the symmetry operation \(h \rightarrow -h\), while the nonlinear term \(\Psi\) has the opposite parity from that of \(\partial^2 h/\partial x^2\). Therefore, \(<\Psi_c(\partial^2 h/\partial x^2)_c> = 0\). In contrast, one can easily show that the remaining linear discrete diffusion term \(\Gamma\) approaches \((\partial^2 h/\partial x^2)_c\) at sufficient coarse graining. Hence we get from Eq. (9) that \(\nu = \nu_0\) confirming our previous arguments.

We now re-examine the conventional discretization in Eq. (2) in light of our new results. In this case, the interface distribution \(P[h]\) has no simple solution in general. An exception is the linear \(\lambda_0 = 0\) case in which Eqs. (2) and (3) become identical. Then Eq. (8) is again the exact steady state solution and we have \(\nu = \nu_0\), \(D = D_0\) and \(\lambda = \lambda_0 = 0\). A finite \(\lambda_0\) perturbs the system. We found numerically at \(\lambda_0 = 3\) and \(\nu_0 = D_0 = 1\) that the interface distribution \(P[h]\) is not far from that in Eq. (8). However, there is a small skewed correlation among the height differences of neighboring lattice points which can be exemplified by a skewness in the probability distribution of \(\Gamma_i\) defined in Eq. (5). As a result, the up-down symmetry of \(P[h]\) is broken and Eq. (9) now gives \(\nu = \nu_0 + <\Psi_c(\partial^2 h/\partial x^2)_c> / <(\partial^2 h/\partial x^2)_c^2> \neq \nu_0\). The proof of \(D = D_0\) is similar to the previous case. Our numerical results favor a slightly larger \(\lambda\) than \(\lambda_0\) instead of an equality. It can be caused by some non-trivial dependence of \(P[h]\) on the inclination in contrast to that for the new discretization.

The new discretization is also a valuable tool for numerical investigations. Realizations of steady state interfaces could be generated directly using the exact distribution in Eq. (8). To simulate the dynamics, the equations can be integrated using Euler’s method which has an error \(\mathcal{O}(\Delta t^{1/2})\) for stochastic equations [9]. However, an operator splitting approach is far more efficient. Each iteration now consists of two half steps:

\[
h^{n+\frac{1}{2}} = U_L[h^n, \Delta t] \tag{10}
\]
\[
h^{n+1} = U_N[h^{n+\frac{1}{2}}, \Delta t] \tag{11}
\]

where \(U_L\) acting on \(\{h^n_i\}_{i=1}^L\) is the stochastic linear evolution operator for \(\Gamma\) and \(\eta\) only in Eq. (4), while \(U_N\) is the nonlinear evolution operator for the remaining \(\Psi\) term. By noting
that $P[h]$ in Eq. (8) is also the steady state solution of both $U_L$ and $U_N$ independently, it is easy to show that the continuum parameters $c$ and $\lambda$ and the short time parameters $\nu$ and $D$ derived above remain exact. Hence the relevant dynamics is not perturbed despite an $O(\Delta t^{1/2})$ error in the particular realization of the interface. The linear operator $U_L$ can be handled exactly and Eq. (10) implies, after some algebra,

$$h_{i}^{n+\frac{1}{2}} = \sum_{j=1}^{L} K_{i-j}^{\Gamma} h_{j}^{n} + \sqrt{2D_0\Delta t} \sum_{j=1}^{L} K_{i-j}^{\eta} \xi_{j}^{n}$$

(12)

where the $\xi_j$'s are independent standard Gaussian variables. The propagators $K^{\Gamma}$ and $K^{\eta}$ are computed from their Fourier coefficients:

$$\tilde{K}_{k}^{\Gamma} = \exp(-\gamma_{k}\Delta t)$$

(13)

$$\tilde{K}_{k}^{\eta} = \begin{cases} 1 & \text{if } k = 0 \\ \left\{ \left[ 1 - \exp(-2\gamma_{k}\Delta t) \right] / (2\gamma_{k}\Delta t) \right\}^{1/2} & \text{if } k \neq 0 \end{cases}$$

(14)

where $\gamma_{k} = \cos(2\pi k/L)$ and $k$ is an integer from 0 to $L-1$. In practice, the propagators are sharply peaked so that summation over only $|i-j| \leq 5$ in Eq. (12) is sufficient. The deterministic evolution in Eq. (11) can be integrated using the fourth-order Runge-Kutta method with an error $O(\Delta t^4)$ which is also the overall error of our approach.

To test the numerical stability, we simulate initially flat interfaces of size $L = 128$ at $\nu_0 = D_0 = 1$ with various values of $\lambda_0$ each for a period $10000/\lambda_0$. Figure 3 plots $\Delta t_c$ against $\lambda_0$ where $\Delta t_c$ is the critical time step just small enough to ensure stability during a run. For the new discrete equations integrated using the operator splitting Runge-Kutta approach and Euler’s method, we found respectively $\Delta t_c \sim \lambda_0^{-0.89}$ and $\Delta t_c \sim \lambda_0^{-1.76}$ for $\lambda_0 \gtrsim 1$. For the conventional approach of Euler’s algorithm in Eq. (2), the result is initially similar to that of the same method applied to the new discretization. However, $\Delta t_c$ drops faster than exponentially at $\lambda_0 \gtrsim 8$. We suspect that there is a critical $\lambda_0$ beyond which instability is unconditional. For Euler’s method, $\Delta t_c = 0.5$ at $\lambda_0 \lesssim 1$ because of an instability of the diffusive term [11]. The above findings should be important for further understanding of numerical instabilities in equations for interfaces. The superior
performance of our discretized equations when integrated with the operator splitting method is evident. The exponent $-0.89$ in fact represents a surprisingly good stability, taking into account that the dynamic time scale of the interface is proportional to $\lambda_0^{-1}$ for large $\lambda_0$. Besides improved stability, it is about 30 times faster than the conventional approach for example at $\lambda_0 = 3$ for a small systematic error of less than $0.05\%$ in the average growth velocity $c$.

The KPZ equation can be recast using a Hope-Cole transformation into a form which describes directed polymers in random media. It has been reported in Refs. [12] and [3] that the discretized versions of the transformed equation are numerically more stable than those obtained directly from the KPZ equation. Yet, our numerical work shows that their stability and hence the computational efficiency is only in between those of the conventional and our new discrete equations in 1+1 dimensions. These discretizations also suffer from the shortcoming that the effective diffusion coefficient is incompatible with the nominal value. Nevertheless, these methods work also in higher dimensions while it is not clear how our discretization can be generalized.

In conclusion, we have explained that the conventional finite difference approach does not provide a genuine direct numerical integration of the KPZ equation since the continuum diffusion coefficient is incompatible with the nominal one in the discrete equations. This is explained by the microscopic roughness and skewness of the interface at steady state. Despite this anomaly, the discrete equations themselves are in the KPZ universality class and thus the scaling exponents measured in previous works are all valid. A novel discretization for the KPZ equation is studied. The continuum diffusion coefficient is hence shown analytically to be equal to the nominal value. However, this equality is due to subtle cancelation of terms in the Fokker-Planck equation and should not hold in general. This letter has focused on the KPZ equation in 1 + 1 dimensions. However, the conventional finite difference integration approach is also routinely applied to growth in higher dimensions as well as to variants of the KPZ equation and related problems such as the Kuramato-Sivaskinsky equation, etc. [1]. It should be interesting to examine limitations of those results in light of our findings. There
are few investigations on the generalization of the KPZ equation with higher order terms [5], although they may be necessary for successful renormalization group calculations [13]. Our refined understanding on the integration approach should be important for generating such higher order terms in a controlled manner.

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FIG. 1. Snapshots of a segment of an interface generated by numerical integration. The time between two consecutive snapshots is 0.2 corresponding to 20 iterations.
FIG. 2. Inverse method results on the continuum parameters $\lambda$, $\nu$ and $D$ as functions of the spatial and temporal resolutions $l$ and $\tau$ respectively. The dotted lines are $\lambda = 3.04$ and $\nu = 1.14$. 
FIG. 3. Largest possible time step $\Delta t_c$ for numerical stability against $\lambda_0$ for Eq. (4) integrated respectively by operator splitting approach (□) and Euler’s method (○), and for Eq. (2) integrated by Euler’s method (×).