Numerical Simulation and the Universality Class of the KPZ Equation for Curved Substrates

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The Kardar-Parisi-Zhang (KPZ) equation for surface growth has been analyzed for over three decades, and its properties and universality classes are well established. The vast majority of all the past studies were, however, concerned with surface growth that started from flat substrates. In several natural phenomena, as well as technological processes, interface growth occurs on curved surfaces. Examples include tumor and bacterial growth, as well as the interface between two fluid phases during injection of a fluid into a porous medium in which it moves radially. Since in growth on flat substrates the linear size of the system remains constant, whereas it increases in the case of growth on curved substrates, the universality class of the resulting growth process has remained controversial. Some experiments indicated the same power-law scalings of the interface width, \( w(t) \sim t^\beta \), as in the case of growth on planar surface. Escudero (Annal. Phys. 324, 1796, 2009) argued, on the other hand, that for the radial KPZ equations in (1+1)-dimension, the interface width should increase as \( w(t) \sim \ln(t) \) in the long-time limit. Krug (Phys. Rev. Lett. 102, 139601, 2009) argued, however, that the dynamics of the interface must remain unchanged with a change in the geometry. On the other hand, other studies indicated that for radial growth the exponent \( \beta \) should remain the same as that of the planar case, regardless of whether the growth is linear or nonlinear, but that the saturation regime will not be reached anymore. We present the results of extensive numerical simulations in (1+1)-dimensions of the KPZ equation, starting from an initial circular substrate. We find that unlike the KPZ equation for flat substrates, the transition from linear to nonlinear universality classes is not sharp. Moreover, the interface width exhibits logarithmic growth with the time, instead of saturation, in the long-time limit. Furthermore, we find that evaporation dominates the growth process when the coefficient of the nonlinear term in the KPZ equation is small, and that average radius of interface decreases with time and reaches a minimum but not zero value.

I. INTRODUCTION

Introduction. Surface growth is a phenomenon common to many processes of fundamental scientific interest and practical applications, which occurs over a broad range of length scales, ranging from nanometers in biological growth [1] and fabrication of thin films [2], to meters or larger in fluid flow in porous media [3]. Therefore, the physics of interface growth and the mechanisms that contribute to it have been studied for a long time [4, 5] by experiments, theoretical analysis, and numerical simulations. In particular, interface dynamics has been studied with both discrete and continuum models. The discrete models are governed by growth rules that are set such that they produce the interface dynamics and growth in the phenomena of interest. For example, to model surface deposition the positions of the newly added particles are selected based on the state of their neighboring particles in order to identify the most stable landing positions for them. On the other hand, if the growth phenomenon is to be studied at large length scales, the process is modeled by continuum models represented by stochastic differential equations [4, 5]. Scaling analysis of such phenomena is also very useful, since regardless of the system’s details, their dynamics can be characterized by power laws and universality classes. In particular, one of the most important properties of a growing surface is the interface width \( w(t) \), defined by

\[
    w(t) = \left( \langle h^2 \rangle - \langle h \rangle^2 \right)^{\frac{1}{2}}. \tag{1}
\]
where \( h(x, t) \) is the height of the surface at position \( x \) at time \( t \), and \( \langle \cdot \rangle \) indicates its average over various positions. For most growth phenomena that start from a flat substrate, the width \( w(t) \) follows the Family-Vicsek scaling law \([6]\):

\[
w(t) \sim \begin{cases} t^\beta & t < t_x \\ L^\alpha & t > t_x \end{cases}
\]

in which \( \alpha \) and \( \beta \) are, respectively, the roughness and growth exponents, and \( t_x \) is a cross-over time, the time at which a transition occurs from growth to the saturation regime in which \( w(t) \) no longer grows with time.

One of the most successful continuum models for describing a wide range of interface growth is the Kardar-Parisi-Zhang (KPZ) equation \([4, 7]\):

\[
\frac{\partial h(x, t)}{\partial t} = \nu \nabla^2 h(x, t) + \frac{\lambda}{2} \left[ \nabla h(x, t) \right]^2 + F + \eta(x, t), \tag{3}
\]

in which \( F \) is the constant flux of incoming particles (velocity of the height growth), \( \nu \) is the surface tension, \( \lambda \) is a parameter of the model, and \( \eta \) represents thermal fluctuations of the incoming flux with the statistical properties:

\[
\langle \eta(x, t) \rangle = 0, \tag{4}
\]

\[
\langle \eta(x, t) \eta(x', t') \rangle = 2D \delta(x - x') \delta(t - t'). \tag{5}
\]

In many cases, one can choose a reference frame that moves in the growth direction with a constant velocity equal to the growth rate of the average height \( \langle h \rangle \), as a result of which equation (3) reduces to

\[
\frac{\partial h(x, t)}{\partial t} = \nu \nabla^2 h(x, t) + \frac{\lambda}{2} \left[ \nabla h(x, t) \right]^2 + \eta(x, t). \tag{6}
\]

Equation (6) is the simplest nonlinear model of interface growth, and is considered as the standard model of the phenomenon over the last three decades. Ignoring the nonlinear term reduces Eq. 6 to the linear model of Edwards and Wilkinson (EW), which in the case of growth on a flat substrate can be solved, resulting in, \( \beta = (2 - d)/4 \) and \( \alpha = (2 - d)/2 \), for \( d \)-dimensional growth. Unlike the EW equation, however, due to its non-linearity the solution of the KPZ equation is not available in all dimensions. In \((1+1)\)-growth on a line, the exact values, \( \alpha = 1/2 \) and \( \beta = 1/3 \) have been obtained through scaling analysis and by renormalization group methods \([4]\), as well as by random-matrix theory \([8]\). In higher dimensions, however, the exponents can not be determined analytically and, therefore, numerical solutions must be used.

In many natural phenomena, as well as technological processes, interface growth occurs on curved surfaces, such as cylindrical and spherical surfaces. Examples include tumor \([9, 10]\) and bacterial growth, as well as the interface between two fluid phases in, for example, injection of a fluid into a porous medium in which growth occurs radially. There are some fundamental differences between such processes and those that have been studied so far for growth starting from flat surfaces. A main difference is that in growth on a flat substrate, the linear size of the system - the end-to-end distance between the boundaries - remains constant with time during the process, whereas it increases in the case of growth on curved substrates \([11]\).

In order to deal with such a difference, enlarging substrates have been modeled and studied \([12–15]\). One of the most important issues arising in such a problem is whether such differences affect the scaling properties of the growth process. In order to address the issue, one must solve the KPZ equation in cylindrical or spherical geometry, with the appropriate initial and boundary conditions. To rewrite the KPZ equation in a form suitable for a curved substrate, Maritan et al. \([16]\) presented a parametrization-independent form of the equation, from which one obtains the equation for radial growth in \((1+1)\)-dimension, given by \([16–19]\)

\[
\frac{\partial R(\theta, t)}{\partial t} = \frac{\nu}{R(\theta, t)} \frac{\partial^2 R(\theta, t)}{\partial \theta^2} - \frac{\nu}{R(\theta, t)} R(\theta, t) + F + \frac{F}{2R(\theta, t)^2} \left[ \frac{\partial R(\theta, t)}{\partial \theta} \right]^2 + \frac{1}{\sqrt{R(\theta, t)}} \eta(\theta, t), \tag{7}
\]

in which \( R(\theta, t) \) is the angle- and time-dependent radius, and \( \eta(\theta, t) \) is the uncorrelated thermal
noise that follows the same statistics as in Eqs. (4) and (5), with $x$ replaced by $\theta$.

Some efforts have been made to understand the dynamical behavior of the radial KPZ equation. For example, some experiments have indicated the same power-law scalings as in the case of growth on planar surface [20], but the issue remains unresolved. Escudero [17] presented some analytical conjectures and argued that for the radial EW and KPZ equations in $(1+1)$-dimension, the interface width increases as $w(t) \sim [\ln(t)]^{1/2}$ in the long-time limit, $t \gg t_\times$, in contrast to the planar case. Krug [21] argued, however, that the dynamics of the interface must remain unchanged with a change in the geometry. On the other hand, other studies [22, 23] indicated that for radial growth the exponent $\beta$ should be the same as that of the planar case, regardless of whether the growth is linear or nonlinear, but that the saturation regime will not be reached anymore because the mean radius of the interface increases with higher speed than the correlation length. These works employed asymptotic analysis in combination with simple discrete models, such as the Eden model, and radial growth was introduced by enlarging with time the lattice at the interface position. In addition, some numerical works have also been carried out. Batchelor et al [19] introduced a form of the KPZ equation that exhibited the power law $t^\beta$ of Eq. (2), with the same exponent as in the planar growth, while Carrasco et al [24] investigated numerically the radial EW equation, which seemed to support the $[\ln(t)]^{1/2}$ behavior predicted by Escudero.

It is clear that the nonlinear term of the KPZ equation plays a critical role in determining its scaling properties. There are two fixed points in the renormalization group analysis of the KPZ equation in the Cartesian coordinates, with one corresponding to $\lambda = 0$, and a second one associated with $|\lambda| > 0$. The former is a repelling fixed point, whereas the latter is an attractive one, indicating that the growth dynamic belongs to the usual KPZ universality class for any nonzero $\lambda$. To determine the true behavior of radial KPZ equation, especially in the long-time regime, we have solved the equation numerically in $(1+1)$-dimension, growing the interface on a circular substrate, and investigated the role of the nonlinear term of the equation in order to determine whether, similar to the planar growth, it controls the transition between various universality classes.

Since the KPZ contains several parameters, we first reduce their number by introducing dimensionless variables:

\[
\tilde{R} = R\left(\frac{\nu}{D}\right),
\]

\[
\tilde{t} = t\left(\frac{\nu^3}{D^2}\right),
\]

\[
\lambda = F\left(\frac{D}{\nu^2}\right).
\]  

Rewriting the radial KPZ equation (7) using (8) and deleting the tilde lead to the following equation

\[
\frac{\partial R(\theta, t)}{\partial t} = \frac{1}{R(\theta, t)^2} \frac{\partial^2 R(\theta, t)}{\partial \theta^2} - \frac{1}{R(\theta, t)} + \lambda + \frac{\lambda}{2R(\theta, t)} \left(\frac{\partial R(\theta, t)}{\partial \theta}\right)^2 + \frac{1}{\sqrt{R(\theta, t)}} \eta(\theta, t),
\]  

which can be solved numerically by the finite-difference (FD) and finite-element (FE) methods.

\[
R_i^{n+1} - R_i^n = \frac{1}{(R_i^{n+1})^2} \left[ R_i^{n+1} - 2R_i^{n+1} + R_i^{n+1} \right] \\
- \frac{1}{R_i^{n+1}} + \lambda + \frac{\lambda}{2(R_i^{n+1})^2} \left[ R_i^{n+1} - R_i^{n+1} \right]^2 \\
+ \frac{\sqrt{\lambda}}{\sqrt{\Delta t}} \frac{\xi_i}{R_i^{n+1}},
\]  

In the FD method we discretized both time and space variables with fully-implicitly discretization, which results in the following discretized
where \( n \) and \( i \) are, respectively, the time step, and the node numbers, and \( \xi_i \) is a random number attributed to node \( i \), generated by the Box-Muller algorithm\([25]\). The number of grid points were 1024, and the time step was 0.2. In order to reduce the noise in the results 100 realizations were generated and the results were averaged over them. Equation (10) represents a system of nonlinear equations, which we solved by the Newton’s and bi-conjugate gradient methods.

To further check the numerical results obtained by the FD method, we discretized the time via the forward Euler method and used the conforming FE method to discretize the angular variable \( \theta \). The resulting weak form of the equation in suitable functional space \( V \) (in this case, it is the space of square integrable functions with square integrable first derivative) is as follows,

\[
\begin{aligned}
\left( R^n, \frac{R^{n+1} - R^n}{\Delta t}, v \right) = \\
\left( \frac{\partial R^n}{\partial \theta}, \frac{\partial v}{\partial \theta} \right) + \left( -R^n + \lambda(R^n)^2 + \frac{\lambda}{2} \left( \frac{\partial R^n}{\partial \theta} \right)^2 \\
+ \frac{\sqrt{2}}{\sqrt{\Delta t}(R^n)^{3/2}} \xi_i \right), \quad \forall v \in V ,
\end{aligned}
\]

where \( (,..) \) denotes the inner product in \( V \). In order to discretize the above equation, finite dimensional subspace \( V_n \) of \( V \) is considered. In our case, both test and trial spaces are the finite dimensional space \( V_n = \text{span} \{ \varphi_i \}_{i=1}^N \), where each \( \varphi_i \) is the hat function (piecewise linear polynomials) obtained on the quasi-uniform meshes on the radial line. So the approximation for the unknown is described by,

\[
R^n(\theta) = \sum_{i=1}^N c_i^n \varphi_i(\theta),
\]

where \( N \) denotes the number of the basis functions of which we used 512. The time step and the number of angle segmentations were the same as in the FD method, 0.2 and 1024, respectively. The resulting linear system of equations was solved with the direct LU decomposition method using the LAPACK package \([26]\).

To understand the dynamical behavior of the system, we studied the time evolution of the interface width by solving equation (9) with both aforementioned numerical methods. Two processes play important roles in the determination of the growth dynamics: competition between deposition and evaporation from the interface, and saturation, both of which are controlled by the nonlinear term of the KPZ equation. Lateral growth, which is a result of the nonlinear term, is responsible for the saturation. In growth on a flat substrate, the nonlinear term induces the appearance of correlations perpendicular to the growth direction, which grow with time until the correlation length becomes comparable with the linear size of the substrate. Consequently, the entire system becomes correlated and, as a result, the roughening of the surface stops, i.e., \( w(t) \) saturates. In contrast, on, for example, a spherical substrate, the linear size of the system increase with the growing average height of the surface, the radius of the sphere. Therefore, the correlation length can still grow when the system saturates, resulting in very slow growth in \( w(t) \). This is shown in Fig. 1. We find, based on the inset of Fig. 1, that, in the long-time limit the growth is logarithmic, hence supporting the prediction by Escudero and others \([11, 17]\).

![Figure 1. Logarithmic plot of interface width \( w \) as a function of time. The fitted curve represents a power law, shown to indicate that the early stages of growth process is indeed governed by a power law. Unlike growth on flat substrates, however, the growth process will continue after saturation, with its speed being very small. This is shown in the inset, which is a plot of \( w \) as a function of \( \sqrt{\ln t} \).](image-url)
numerical value of the growth exponent $\beta$, we fitted $w(t)$ to a power law at relatively short times, shown in Fig. 1. The results are shown in Fig. 2, which presents dependence of $\beta$ on the nonlinear coefficient $\lambda$ for two cases, one when the constant term in equation 9, which represents an external driving force, takes on several nonzero values, and the second case when it is zero. In both cases $\beta \approx 1/4$ when $\lambda$ is small enough (but not necessarily 0), then it approaches $1/3$ as $\lambda$ increases. Therefore, unlike the behavior of the KPZ equation in the Cartesian geometry, the boundary between the linear and nonlinear universality classes is not sharp, rather the system transitions smoothly from the linear universality class to the nonlinear one as $\lambda$ increases. When $\lambda$ is larger than a certain value, however, the system is in the usual KPZ universality class. The transition between these two regimes depends, however, on the existence of the nonvanishing term $\lambda$. We will return to this point shortly.

![Figure 2](image)

**Figure 2.** Growth exponent $\beta$ as a function of the coefficient of nonlinear term $\lambda$, computed by numerical simulation of Eq. 9.

Another process in surface growth is the competition between deposition - adding particles to the interface - and evaporation - removing particles from the growing surface. This process too is controlled by the nonlinear term of the KPZ equation. On a flat substrate, positive values of $\lambda$ represent the case in which the number of newly deposited particles on the interface is on average more than those of leaving it, which leads to positive growth in the average height $\langle h \rangle$, even in the absence of the external driven force. In contrast, negative value of $\lambda$ implies evaporation takes out more particles than the number particles added by deposition, resulting in negative growth (shrinking) of $\langle h \rangle$.

On the other hand, positive value of $\lambda$ in spherical growth does not necessarily result in increasing $\langle h \rangle$. This is shown in Fig. 3 that presents plots of both the average radii of the interface $\langle R \rangle$ and the interface width $w$ as functions of time for a positive but relatively small value, $\lambda = 10^{-3}$. Here, $\langle R \rangle$ is equivalent to $\langle h \rangle$ in growth on flat substrate. It is clear that surface thickness decreases with time until it reaches a nonzero minimum value. The top right inset in Figure 3 is a zoomed-in view of $\langle R \rangle$ at the transition point. The interface width has its usual power-law growth before this transition point, but it suddenly drops to a relatively small value at the transition point and, then, fluctuates around it.

To understand the transition better, we plotted two snapshots of the interface, one at a time earlier than the transition - the inset on the left side of Fig. 3 - and the other one after the transition - the right bottom inset. Before the transition, the interface has a usual roughness profile, as reported in many of numerical simulation of the KPZ equation. The morphology of the interface is, however, very smooth at times after the transition. A remarkable point of the growth process at this point is that both $\langle R \rangle$ and $w$ reach a fixed point and fluctuate around it. Even thermal noise does not play any role in this case, as it cannot make any significant change in either the morphology of interface or in its average height.

![Figure 3](image)

**Figure 3.** Plot of interface width $w$, as well as average interface diameter $\langle R \rangle$, versus time for $\lambda = 10^{-3}$. The top right inset plot is a zoomed-in part of $\langle R \rangle$ at the transition point. The other two inset plots are snapshots of the interface at times before (left) and after (right) the transition point.
As mentioned earlier, the transition between evaporation- and deposition-dominated regimes occurs at some finite value, \( \lambda = \lambda_t \), which depends on the curvature of the substrate \( R_0 \). This is shown in Fig. 4, which presents \( \lambda_t \) as a function of the inverse of substrate curvature for two cases, one in Fig. 4(a) without the constant term, and one with a nonzero term in Fig. 4(b). They both appear to be linear functions of \( 1/R_0 \) and, therefore, were used to obtain the asymptotic value for a flat substrate, the limit \( R_0 \to \infty \). We obtained, \( \lambda_t \to 0 \) as \( R_0 \to \infty \), indicating that in the asymptotic limit, \( R_0 \to \infty \), Eq. 9 becomes equivalent to the usual KPZ equation. In contrast, when the constant term is dropped out, the asymptotic value is \( \lambda_t \approx 3 \), which differs from that of the standard KPZ equation.

To explain the difference between the two cases, we refer to the role of constant term in the standard KPZ equation. Ignoring the constant term in growth on a flat substrate implies that an observer is on the reference frame, moving with a constant velocity, but viewing it on a reference frame that is fixed on the substrate results in the same observations. In the case of the growth on a curved substrate, however, ignoring the constant term does not imply a reference frame moving with the average growth velocity, hence it provides a different vision for the interface dynamics.

To determine the universality class to which the time-evolution of Eq. 9 belongs, one needs to compute both the growth exponent \( \beta \) and the roughness exponent \( \alpha \). The latter was computed using the height-height correlation function:

\[
C(\theta_1 - \theta_2) = \langle [R(\theta_1) - R(\theta_2)]^2 \rangle
\tag{13}
\]

where \( \langle \cdot \rangle \) indicates on average over the thermal noise. \( C(\theta) \) has the following power-law form,

\[
C(\theta) \sim \theta^{2\alpha}
\tag{14}
\]

where \( \alpha = 1/2 \) for the standard KPZ equation [4, 7, 28]. Figure 5 is a typical plot of correlation function versus \( \theta \) at the final stage of simulation for computing the roughness exponent.

The results of the fitting are listed in Table I for both cases of with or without the constant term. In both cases, when \( \lambda > \lambda_t \), the roughness exponent is compatible with that of the standard KPZ equation. On the other hand, \( \alpha \approx 1 \) when \( \lambda < \lambda_t \), indicates a completely correlated and smooth interface, as shown in the right bottom inset of Fig. 3. When considering the constant term, \( C(\theta) \) reaches its flattening regime at very small \( \theta \), leaving a very small set of data for fitting. This means estimating \( \alpha \) is problematic and, consequently, we do not present the results.
for $\lambda > 1$.

| $\lambda$ | $2\alpha$ with constant term | $2\alpha$ without constant term |
|-----------|-----------------------------|---------------------------------|
| 0.001     | 1.99                        | 1.99                            |
| 0.01      | 1.02                        | 1.99                            |
| 0.1       | 0.95                        | 1.99                            |
| 1         | 0.87                        | 1.99                            |
| 3         | ...                         | 1.99                            |
| 5         | ...                         | 1.99                            |
| 7         | ...                         | 0.98                            |
| 9         | ...                         | 1.10                            |
| 10        | ...                         | 1.00                            |

Table I.

**Outlook.** The vast majority of the previous studies of the KPZ equation for surface growth over the past three decades were concerned with surface growth that began from flat substrates. In several natural phenomena, as well as technological processes, such as tumor and bacterial growth, as well as the interface between two fluid phases during injection of a fluid into a porous medium, interface growth occurs on curved surfaces. Since in growth on flat substrates the linear size of the system remains constant, whereas it increases in the case of growth on curved substrates, the universality class of the resulting growth process has remained controversial, with conflicting results reported by various groups. In this paper we presented the results of extensive numerical simulation in (1+1)-dimensions of the KPZ equation, starting from an initial circular substrate. Our results indicate that, unlike the KPZ equation for flat substrates, the transition from linear to nonlinear universality classes is not sharp. Moreover, the interface width exhibits logarithmic growth with the time, instead of saturation, in the long-time limit. In addition, the simulations indicate that evaporation dominates the growth process when the coefficient of the nonlinear term in the KPZ equation is small, and that average radius of interface decreases with time and reaches a minimum but not zero value. Thus, while there are certain similarities between surface growth on flat and curved surfaces, there are also significant differences.

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