Large-scale simulations of ballistic deposition: The approach to asymptotic scaling

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Extensive kinetic Monte Carlo simulations are presented for ballistic deposition (BD) in (1 + 1) dimensions. Asymptotic scaling is found only for lattice sizes \( L \gtrsim 2^{12} \). Such a large system size for the onset of scaling explains the widespread discrepancies of previous reports for exponents of BD in one and likely higher dimensions. The exponents obtained from our simulations, \( \alpha = 0.499 \pm 0.004 \) and \( \beta = 0.336 \pm 0.004 \), are in excellent agreement with the exact values \( \alpha = \frac{1}{3} \) and \( \beta = \frac{1}{3} \) for the one-dimensional Kardar-Parisi-Zhang equation. Our findings make possible a more informed exploration of exponents for BD in higher dimensions, accurate estimates of which have proven to be elusive.

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Fluctuations of growing surfaces are often described by idealized models [1–3] wherein the complex interactions between atoms or molecules are replaced by simple transition rules on a lattice that abstract the essence of these interactions. The appeal of such models stems from the fact that their rules can be easily implemented in efficient kinetic Monte Carlo (KMC) algorithms. This enables a comprehensive analysis of their statistical characteristics, which can be compared directly with experiments [4–6].

A complementary approach is based on postulating a stochastic differential equation. Solutions of such equations typically focus on the asymptotic kinetic roughening regime, where the standard deviation \( W(L,t) \) of the surface profile exhibits dynamic scaling [7]:

\[
W(L,t) = [(\langle h^2 \rangle - \langle h \rangle^2)^{1/2}] \sim L^\alpha f(t/L^\beta).
\]

(1)

Here \( h(x,t) \) is the surface height at position \( x \) and time \( t \), \( L \) is the lateral viewing scale, \( \alpha \) is the roughness exponent, \( z \) is the dynamic exponent, and \( f \) is a scaling function. At early times (\( t \ll L^2 \)), \( f(x) \sim x^{\alpha/\beta} \) and \( W \sim t^\beta \), where \( \beta \) is the growth exponent and \( z = \alpha/\beta \). For long times (\( t \gg L^2 \)), \( f \rightarrow \) constant, so the saturated roughness \( W_{\text{sat}} \sim L^\alpha \). The connection to a lattice model is based on comparing exponents and invoking universality [2].

The foregoing paradigm can be justified for many models [2,8], but outstanding issues persist in some cases, most notably, ballistic deposition (BD). Originally formulated as a model for aggregation and sedimentation [9,10], BD is the prototypical model of nonconserved growth, in which the volume of material over the substrate is not equal to that deposited, in this case because of void formation. In classic BD [9,10] a particle impinges on a randomly chosen lattice site and irreversibly attaches to the first vertical or lateral nearest neighbor encountered. The updating algorithm for the integer heights \( h_i(n) \) at site \( i \) after \( n \) depositions is

\[
h_i(n+1) = \max \{h_{i-1}(n), h_i(n) + 1, h_{i+1}(n)\}.
\]

(2)

for \( i = 1, 2, \ldots, L \), where \( \max \{x, y, z\} \) yields the maximum of the three arguments.

The continuum formulation of BD is thought to be the Kardar-Parisi-Zhang (KPZ) equation [11],

\[
\frac{\partial u}{\partial t} = \nu \nabla^2 u + \lambda(\nabla u)^2 + \xi,
\]

(3)

where \( u(x,t) \) is the deviation of the height from its mean at position \( x \) and time \( t \) on a \( d \)-dimensional surface, \( \nu \) is the surface tension, \( \lambda \) is the “excess velocity” [2], and \( \xi \) is a Gaussian noise with mean zero and covariance,

\[
\langle \xi(x,t)\xi(x',t') \rangle = 2D\delta(x-x')\delta(t-t').
\]

(4)

Although among the first surface growth models to be studied with KMC simulations [7], discrepancies remain between the scaling properties of BD and the KPZ equation [12–14], even on one-dimensional (1D) surfaces. Their relationship is even less certain in higher dimensions [15–27], including the suggestion [28] that the two models belong to different universality classes.

In this Rapid Communication, we report the results of extensive KMC simulations of BD on 1D lattices with up to \( 2^{20} \) sites, well beyond the onset of saturation, for up to \( 10^6 \) independent realizations. In view of the pitfalls associated with hidden correlations in random number generators [29], which may be especially acute for BD [13], we have used the Mersenne twister MT19937 [30,31]. This pseudorandom number generator has a period of \( 2^{19937} - 1 \), output that is uniformly distributed in 623 dimensions, implying negligible serial correlation, and has passed the most stringent statistical tests [32]. These properties, and its computational efficiency, make the Mersenne twister eminently suitable for large-scale KMC simulations.

The massive computational resources required for the simulations reported here relied upon unconventional “overnight office computing.” Social networking skills were employed in the development of the Simulation Through Social Networking (STSN) project, in which 120–130 computers were utilized for some 9 months to drive the KMC simulations of even the largest lattices deep into the saturation region [33]. Details may be found in Refs. [36,37].
Figure 1 shows a log-log plot of $W_{\text{sat}}$ against $L$ using the data in Table I. $W_{\text{sat}}$ was calculated by taking samples every $4\tau$ to $\tau$ monolayers (MLs), depending on the lattice size, where $\tau \sim L^{3/2}$ is the relaxation time [38], to ensure that the data points were statistically independent, and taking binned horizontal averages to alleviate any drift in the data over time $[2,39]$. Simulations for $L = 16\,384$, $L = 32\,768$, and $L = 65\,536$ were carried out for up to $33.5 \times 10^9$ layers, but many data points were excluded because of the stretched exponential tail in $W_{\text{sat}}$. Stretched exponential tails have also been observed in the dynamical structure factor in the stationary regime of the $1+1$-dimensional KPZ equation $[40,41]$.

Most apparent from Fig. 1 is that an accurate estimate of $\alpha$ requires system sizes beyond $L = 211$ because of the slow approach to asymptotic scaling. For the smallest systems there is appreciable deviation from the asymptotic behavior because of finite-size effects which persist even to system sizes of $2^{11}$. Our estimate of

$$\alpha = 0.499 \pm 0.004,$$

obtained from the fit between $L = 2^{12}$ and $L = 2^{16}$, captures the value of $\alpha = \frac{1}{3}$ for the 1D KPZ equation $[11]$. To our knowledge, this is the first time that the roughness exponent of BD has been shown to agree with the KPZ value (within the error bounds) directly from an analysis of simulation data and without invoking any scaling corrections $[2,14,28]$. To put our results into perspective, the line from $L = 2^4$ to $L = 2^{12}$ in Fig. 1 indicates the approximate range and slope of the simulation data used in previous work for calculating $\alpha$, resulting in an appreciable underestimate of this exponent.

The slow approach of $\alpha$ to its asymptotic value suggests that a similar trend should be expected for $\beta$. However, in contrast to the calculation of $\alpha$, which requires simulations that extend well into the saturation regime to obtain accurate values of $W_{\text{sat}}$, the problem in determining $\beta$ is not computational overhead per se. Rather, the difficulty lies in precisely delineating the limits of the growth region $[14]$ over which $W \sim t^\beta$.

The growth times $t_\tau$ and the corresponding $\beta_L$ are compiled in Table II. The most striking trend in these data is the slow approach to the asymptotic value $\beta = \frac{1}{3}$ $[11]$, which is even more pronounced than that in Fig. 1. Lattice sizes in excess of $2^{18}$ are needed to obtain $\beta_L$ to within $1\%$ of the exact value.

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These observations can be quantified by fitting the data to the scaling form [14]:

$$\beta_L = \beta + \frac{A}{L^\lambda}.$$  \hfill (6)

The data in Table II yield (Fig. 2) \(A = -0.530 \pm 0.128, \lambda = 0.324 \pm 0.043\), and

$$\beta = 0.336 \pm 0.004$$  \hfill (7)

for \(L = 2^{10} - 2^{17}\). The data for the largest lattices were excluded from this fitting because of insufficient accuracy, but the best fit still lies within their error bars.

In measuring \(t_g\), we have expanded the criteria suggested by Reis [14] by using floating “beginning” and “end” points for each lattice size and imposing a maximum time criterion. Figure 3 shows a log-log plot of \(t_g\) against \(L\) with a linear fit of the data points from \(L = 2^{16}\) to \(L = 2^{20}\). Only when the slope of this line, which we call the “growth-time exponent” \(\gamma\), reaches unity can we say that the systems have reached the asymptotic regime. The power-law growth regime is bounded by (i) the (largely \(L\)-independent) transient regime, during which the system first follows random deposition, before the BD rules determine the growth characteristics, and (ii) the approach to the saturation regime, which is strongly \(L\)-dependent and corresponds to a deviation from power-law behavior of the surface width. For small system sizes, the transient and saturation regimes are sufficiently close together that the growth exponent deviates significantly from the asymptotic BD value (inset to Fig. 3). However, as \(L\) increases, the time between the transient and saturation regimes increases and eventually becomes sufficiently separated to enable true BD behavior to develop. It is for these values of \(L\) that we observe the slope of unity in Fig. 3.

The scaling relation (1) implies that plots of \(W/L^z\) against \(t/L^\gamma\) for different system sizes “collapse” onto the universal scaling function \(f\). Our estimate of \(z = \alpha/\beta\) from the values of \(\alpha\) in (5) and \(\beta\) in (7) is \(z = 1.485 \pm 0.03\) [42]. The KPZ value of \(z = \frac{1}{3}\) lies within the uncertainty of this estimate. Figure 4 shows the data collapse for \(L = 2^{14}, 2^{15}, 2^{16}\). The values of \(\alpha\) for these sizes are well into the asymptotic regime (Fig. 1) and the corresponding values of \(\beta\) are within \(\sim 0.01\) of the asymptotic value of \(\beta = \frac{1}{2}\) (Table II). We have used our best estimates of \(\alpha = 0.499\) and \(\beta = 0.336\) in this plot, but there are few discernible differences if the exact values are used instead.

The high quality of this data collapse, which is indicative both of the accuracy of our data and the fact that these systems lie within the asymptotic scaling regime, invites a comparison...
with the scaling function of the KPZ model [43]. However, the disparity in the roughness of the surfaces produced by the two models means that the scaling functions are different. This does not preclude the 1D BD model and KPZ equations from belonging to the same universality class, but casts further doubt [28] on the KPZ equation as the continuum expression of BD.

To summarize, we have used massive KMC simulations of BD onto 1D surfaces to demonstrate the slow approach of this system to the asymptotic scaling regime. The exponents $\alpha$ and $\beta$ were shown to converge to the exact values obtained from the KPZ equation, with systems of up to $2^{20}$ sites required for a clear indication of convergence. We have used only a single random generator, the Mersenne twister MT19937, so our results shed no light on the reason for the slow convergence. However, given the long period of this random number generator and its other statistical and operational characteristics, this is likely an intrinsic property of BD. Future work on 1 + 1-dimensional BD will focus on more detailed comparisons between our simulations and numerical solutions of the KPZ equation [41,43].

We conclude with a few remarks about the implications of our results for simulations of BD in higher dimensions. Preliminary simulations on two-dimensional substrates suggest that the slow convergence toward asymptotic scaling persists for higher dimensional substrates, but we have not yet determined the rate of convergence. In this regard, a plot such as Fig. 3 is vital for indicating if a particular system size exhibits statistical characteristics of the asymptotic scaling regime. This will be taken up in a future publication.

B.F. would like to express his deep gratitude to IASBS staff and students for making the STSN project possible. He would also like to thank S. N. Rasuli and especially M. R. Kolahchi for thoughtful discussions.

[33] Social computing is not a new concept. “Volunteer computing” started in the mid-1990s [34] and, by the end of that decade, expanded into the now well-known @home projects in which many thousands of personal computers work together on a single task [35]. STSN is a combination of volunteer and grid computing.
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[38] F. D. A. Aarão Reis, Physica A 316, 250 (2002).
[39] F. D. A. Aarão Reis (private communication).
[42] In fact, we may be able to calculate $\gamma$ from the stationary structure factor, independently of $\alpha$ and $\beta$, as described in Ref. [41] for the KPZ equation.