Large-scale simulations with distributed computing: Asymptotic scaling of ballistic deposition

Bahman Farnudi
Institute for Advanced Studies in Basic Sciences (IASBS), Zanjan 45137-66731, Iran
E-mail: farnudi@iasbs.ac.ir

Dimitri D Vvedensky
The Blackett Laboratory, Imperial College London, London SW7 2AZ, United Kingdom
E-mail: d.vvedensky@imperial.ac.uk

Abstract. Extensive kinetic Monte Carlo simulations are reported for ballistic deposition (BD) in (1 + 1) dimensions. The large system sizes \( L \) observed for the onset of asymptotic scaling (\( L \approx 2^{12} \)) explains the widespread discrepancies in previous reports for exponents of BD in one and likely in higher dimensions. The exponents obtained directly from our simulations, \( \alpha = 0.499 \pm 0.004 \) and \( \beta = 0.336 \pm 0.004 \), capture the exact values \( \alpha = \frac{1}{2} \) and \( \beta = \frac{1}{3} \) for the one-dimensional Kardar-Parisi-Zhang equation. An analysis of our simulations suggests a criterion for identifying the onset of true asymptotic scaling, which enables a more informed evaluation of exponents for BD in higher dimensions. These simulations were made possible by the Simulation through Social Networking project at the Institute for Advanced Studies in Basic Sciences in 2007, which was re-launched in November 2010.

1. Introduction

Ballistic deposition (BD) is a standard model for surfaces driven by the stochastic deposition of new material. Formulated as a model for colloidal aggregation [1, 2], BD is the prototypical model of nonconserved growth, in which the sum (or integral) of heights over the substrate is not equal to the material deposited, in this case because of void formation. The asymptotic behaviour of BD and other models of driven fluctuating interfaces, as exemplified by the variance \( W(L, t) \) of the surface profile, typically exhibit dynamic scaling [3, 4]:

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

(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 (\( t \ll L^z \)), \( f(x) \sim x^\beta \), where \( z = \alpha/\beta \), so \( W \sim t^\beta \). For long times (\( t \gg L^z \)), \( f \to \) constant, so the saturated roughness \( W_{\text{sat}} \sim L^\alpha \).

In one dimension (1D), BD is generally believed to be in the same universality class as the Kardar-Parisi-Zhang equation [5],

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

(2)
where \( u(x, t) \) is the deviation of the height from its mean at position \( x \) and time \( t \) on a \( d \)-dimensional surface, and \( \xi \) is a Gaussian noise with mean zero and covariance

\[
\langle \xi(x, t) \xi(x', t') \rangle = 2D \delta(x - x') \delta(t - t').
\] (3)

Nevertheless, despite being among the first surface growth models to be studied with KMC simulations [3], the past 20 years have seen a wide scatter of estimates for the scaling exponents of BD [4, 6, 7]. In higher dimensions, the relationship between BD and the KPZ equation is considerably more problematic [8–20]. It has even been suggested [7] that BD and the KPZ equation do not belong to the same universality class on substrate dimensions greater than one.

In this paper, we report the results of extensive kinetic Monte Carlo (KMC) simulations for BD on 1D lattices with up to \( 2^{20} = 1,048,576 \) sites, well beyond the onset of saturation for up to \( 10^6 \) independent realisations. This enables us to observe the slow approach to asymptotic scaling in this model and to obtain accurate estimates of the exponents, which agree with those of the KPZ equation. An analysis of these simulations reveals the reason behind the widespread discrepancies in previous reports of exponents for BD and provides a criterion that signifies when a system has entered the asymptotic scaling regime. The latter result enables a more informed exploration of the scaling behaviour of BD in higher dimensions, where simulations are substantially more computationally demanding.

The outline of this paper is as follows. The rules of BD are described in Sec. 2, where we also discuss some of the properties of the surfaces produced by this model. Section 3 provides a brief summary of the Simulation through Social Networking project, which made possible the extensive simulations and the highly accurate results reported in this paper. The estimates for exponents, corrections to scaling, and scaling functions are presented and discussed in Sec. 4. We summarise our findings and draw conclusions in Sec. 5.

2. Ballistic Deposition

In the classical BD model, a particle impinges on a randomly chosen lattice site and irreversibly attaches to the first vertical or lateral nearest neighbour encountered. Figure 1 illustrates how this rule is implemented on a 1D lattice for three types of incident particles. The incident particle A attaches to a lateral nearest neighbour, which results in a void below the attached position. As BD permits no further relaxation, for example, through surface diffusion, this void remains, so the resulting film has porosity. Hence, the volume of this film, as measured by the sum of column heights on each lattice site, exceeds that of the deposited material, i.e. growth is non-conserved. Particles B and C attach to vertical nearest neighbours, so no voids are produced. However, the local height configuration of the deposited position of B will result in voids upon deposition on each adjacent site. The BD rules capture the essence of the sedimentation of small

![Figure 1](image_url). Schematic diagram of BD for three incident particles and their deposition sites (shown shaded). A particle impinges on a randomly chosen site and attaches to the first nearest vertical or lateral nearest neighbour encountered. Particle A attaches to a lateral nearest neighbour, while particles B and C attach to vertical nearest neighbours. As the void between the attached particle A and the surface cannot be filled by any relaxation rules within the model, the film produced by BD has porosity.
material particles under gravity in a liquid [1], or physical and chemical vapour deposition of thin films [21–23].

The updating algorithm of BD on a $d$-dimensional substrate based on the rules in Fig. 1 is expressed in terms of the integer height $h_i(n)$ at lattice position $i$ after $n$ depositions as

$$h_i(n+1) = \max(h_{i-1}(n), h_i(n) + 1, h_{i+1}(n)),$$

for $1 = 1, 2, \ldots, L^d$, where $L$ is the linear size of the system and $\max(x, y, z)$ yields the maximum of its three arguments. The initial conditions are usually taken as a flat substrate, with all heights set equal to zero: $h_i(0) = 0$.

3. Simulation Method

3.1. Simulation through Social Networking

The massive computational resources required for the simulations reported here relied upon unconventional “overnight office computing,” which was developed into a fully-fledged social computing network. Social networking skills were employed in the development of the Simulation through Social Networking (STSN) project, in which 120-130 computers were utilised for some nine months to drive the KMC simulations of even the largest lattices deep into the saturation region.

Social computing is not a new concept. “Volunteer computing” started in the mid-1990s [24] and, by the end of that decade, expanded into the now well-known @home projects in which hundreds of thousands of personal computers work together on a single task [25]. STSN is a combination of volunteer and grid computing. Further details may be found on the project website [26] and in Ref. [27].

The success of STSN relies on exclusivity, quality, and the human touch. STSN operates on the principles characterising a family business, i.e. direct personal contact, customer care, transparency, high quality, and long-term customer retention strategy. Networks are built slowly and carefully to enhance data security through responsible volunteering and to ensure long-term participant involvement through mutual trust and benefit. To this end, a re-launch of the STSN project is currently underway with the cooperation of the students in Information and Communication Technology (ICT) at IASBS as STSN team members and team leaders. The continuity and long-term success of similar projects can be guaranteed only by all-out participation of ICT experts.

3.2. Random Number Generator

In view of the pitfalls associated with hidden correlations in random number generators [28], and the suggestion [29] that BD may be especially sensitive to such correlations, we have used the Mersenne Twister MT19937 random number generator [30, 31]. This pseudorandom number generator has a period of $2^{19937} - 1$, an 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.

4. Results

4.1. The roughness exponent

Figure 2 shows the determination of the roughness exponent $\alpha$ from the slope of a straight-line fit to a log-log plot of $W_{\text{sat}}$ against $L$ for the data in Table 1. $W_{\text{sat}}$ 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 of BD [33], to ensure that the data points were statistically independent, and taking binned horizontal averages to alleviate any drift in the data over time [4]. Simulations
Roughness exponent

\[ \alpha = 0.499 \pm 0.004 \]

**Figure 2.** Log-log plot of \( W_{\text{sat}} \) against \( L \) for the data in Table 1. Error bars are of the order of the symbol size or smaller. The roughness exponent in (5) obtained from the slope of a linear fit over the range \( L = 2^{12} - 2^{16} \) (red dots) is in excellent agreement with the KPZ value of \( \frac{1}{3} \). The broken line indicates the approximate range of simulation data used in previous work (\( L = 2^{4} - 2^{12} \)), which leads to a substantial underestimate of \( \alpha \).

**Table 1.** Saturated roughness \( W_{\text{sat}} \) on 1D lattices of sizes \( L = 2^n \) for \( n = 2, 3, \ldots, 16 \) obtained from KMC simulations with the indicated number of independent realisations. The time to saturation is \( t_x \) and the simulations were continued into the saturation regime for a time \( t_s \). Where none is indicated, the calculated error is smaller than \( 10^{-2} \).

| \( L \) | \( W_{\text{sat}} \) | Error | Realisations | \( t_x \) (MLs) | \( t_s \) (10^6 MLs) |
|-------|-----------------|-------|--------------|----------------|-----------------|
| 4     | 1.33 \( \pm \)  | –     | 100,000      | –              | 4               |
| 8     | 1.97 \( \pm \)  | –     | 100,000      | –              | 1               |
| 16    | 2.63 \( \pm \)  | –     | 93,000       | –              | 1               |
| 32    | 3.40 \( \pm \)  | –     | 100,000      | 19.75          | 1               |
| 64    | 4.41 \( \pm \)  | –     | 10,000       | 44.5           | 1               |
| 128   | 5.82 \( \pm \)  | –     | 10,000       | 108            | 1               |
| 256   | 7.85 \( \pm \)  | –     | 10,000       | 259            | 1               |
| 512   | 10.73 \( \pm \) | –     | 10,000       | 675            | 1               |
| 1,024 | 14.93 \( \pm \) | –     | 7,486        | 1900           | 1               |
| 2,048 | 20.95 \( \pm \) | 0.03  | 1,010        | 5200           | 4.1             |
| 4,096 | 29.39 \( \pm \) | 0.05  | 841          | 13700          | 4.1             |
| 8,192 | 41.58 \( \pm \) | 0.1   | 253          | 38000          | 4.1             |
| 16,384| 58.69 \( \pm \) | 0.2   | 724          | 106500         | 10              |
| 32,768| 84.09 \( \pm \) | 0.2   | 407          | 297000         | 10              |
| 65,536| 116.55 \( \pm \) | 1.0   | 249          | 770000         | 10              |

for \( L = 16, 384 \), \( L = 32, 768 \), and \( L = 65, 536 \) were carried out for up to \( 33.5 \times 10^6 \) layers, but many data points were excluded from the averaging because of the stretched exponential tail in the probability distribution of \( W_{\text{sat}} \) [34].

Most apparent from Fig. 2 is that an accurate estimate of \( \alpha \) necessitates using system sizes beyond \( L = 2^{11} \) because of the slow approach to asymptotic scaling. For the smallest systems there is appreciable deviation from the asymptotic behaviour because of finite-size effects. But even intermediate system sizes \( (L = 2^{9} - 2^{11}) \) adversely affect the estimate of \( \alpha \). 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 \( \alpha = \frac{1}{2} \) for the 1D KPZ equation [5]. 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 any scaling corrections [4,6,7]. To put our results into perspective, the line from $L = 2^4$ to $L = 2^{12}$ in Fig. 2 indicates the approximate range and slope of the simulation data used in previous work for calculating $\alpha$. As these data points and the fit make clear, the use of system sizes smaller than $L = 2^{12}$ results in an appreciable underestimate of $\alpha$.

An alternative method of quantifying the approach to asymptotic scaling, as suggested by Reiss [6], is to first calculate $L$-dependent effective roughness exponents $\alpha_L$, defined by

$$\alpha_L = \frac{\ln[W_{\text{sat}}(L)/W_{\text{sat}}(\frac{L}{2})]}{\ln 2}. \quad (6)$$

These are easily determined from the data in Table 1 and enable the correction-to-scaling form

$$\alpha_L \approx \alpha + AL^{-\Delta}, \quad (7)$$

in which $\Delta$ is a correction-to-scaling exponent and $A$ is a constant. These calculations are not displayed, as the data in Fig. 2 already give a clear indication of the slow approach to asymptotic scaling of BD.

4.2. The growth 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 $W_{\text{sat}}$ (Table 1), the obstacle for determining $\beta$ is not computational overhead per se. Rather, the difficulty lies in delineating the limits of the growth region [6] over which $W \sim t^\beta$. Our results are displayed in Fig. 3 as a plot of $\beta$ against log(1/$L$) of the data compiled in Table 2.

The most striking trend in these data is the slow approach to the asymptotic (KPZ) value of $\beta = \frac{1}{3}$ with increasing system size, which is even more pronounced than that in Fig. 2. Lattice sizes in excess of $L = 2^{18} = 262,144$ are needed to obtain values of $\beta$ to within 1% of the exact value. This observation can be quantified by fitting the data to an expression of the form

$$\beta(1/L) = \beta + a[\log(1/L)]^b, \quad (8)$$

where the asymptotic value is $\beta$, and $a$ and $b$ are fitting parameters. Optimisation over the range from $L = 2^{10}$ to $L = 2^{17}$, as shown in Fig. 4, produces

$$\beta = 0.336 \pm 0.005. \quad (9)$$

\textbf{Figure 3.} Log-linear plot of $\beta$ against log(1/$L$) based on the data in Table 2. The points for the largest lattice sizes (indicated in black) have too few realisations to provide accurate estimates and are included for completeness only. The curve is a fit to the data between $L = 1024$ and $L = 131,072$ of (8). The asymptotic value $\beta = 0.336 \pm 0.005$ obtained from this fit agrees to within errors with the KPZ value of $\alpha = \frac{1}{3}$.
Table 2. The growth exponent $\beta_L$ and the associated error for lattice sizes $L = 2^n$, with $n = 5, \ldots, 20$ obtained from KMC simulations with the indicated number of realisations. The corresponding growth time $t_g$ over which $\beta_L$ is calculated, and its error, are also shown.

| $L$  | $\beta_L$ | Error | Realisations | $t_g$ (MLs) | Error |
|------|-----------|-------|--------------|-------------|-------|
| 32   | 0.176     | 0.01  | 1,000,000    | 2           | 1     |
| 64   | 0.20      | 0.02  | 1,000,000    | 4           | 5     |
| 128  | 0.224     | 0.006 | 1,000,000    | 10          | 5     |
| 256  | 0.254     | 0.002 | 1,000,000    | 20          | 5     |
| 512  | 0.270     | 0.002 | 1,000,000    | 80          | 10    |
| 1,024| 0.280     | 0.002 | 100,000      | 284         | 10    |
| 2,048| 0.2907    | 0.001 | 100,000      | 700         | 10    |
| 4,096| 0.302     | 0.001 | 100,000      | 1,400       | 100   |
| 8,192| 0.308     | 0.001 | 54,000       | 4,200       | 500   |
| 16,384| 0.312    | 0.002 | 810          | 7,936       | 1,000 |
| 32,768| 0.317    | 0.002 | 407          | 23,000      | 7,000 |
| 65,536| 0.322    | 0.0005| 800          | 61,000      | 4,000 |
| 131,072| 0.325   | 0.002 | 105          | 130,000     | 10,000|
| 262,144| 0.323   | 0.01  | 9            | 260,000     | 50,000|
| 524,288| 0.334   | 0.005 | 2            | 520,000     | 100,000|
| 1,048,576| 0.332  | 0.005 | 2            | 1,040,000   | 200,000|

Although the data at the largest lattices (indicated by black symbols in Fig. 3) lack the accuracy for an extrapolation to infinite sizes, and were not included in the fitting, the best fit lies within their error bars. Several ranges of data (including the entire range) were used to fit the above form, and in all cases the asymptotic values of $\beta$ obtained for different fit ranges fluctuate around the KPZ value.

4.3. Correction to scaling
The growth times $t_g$ and the corresponding values of $\beta_L$ are compiled in Table 2. The most striking trend in these data is the slow approach to the asymptotic value of $\beta = \frac{1}{3}$ [5], which is

Figure 4. Effective growth exponents $\beta_L$ plotted against $L^\lambda$ for the data in Table 2 with optimised parameters in the scaling form (10). Only the red points, which correspond to system sizes $L = 2^{10} \cdots 2^{17}$, had large enough growth regions to be included in the fit. The empty red circles, which correspond to $L = 2^{18}$ and $L = 2^{20}$, were excluded from the fit because of insufficient accuracy. The data point corresponding to $L = 2^{19}$ has been omitted for clarity.
even more pronounced than that in Fig. 2. Lattice sizes in excess of $2^{18} = 262,144$ are needed to obtain values of $\beta_L$ to within 1% of the exact value. These observations can be quantified by fitting the data to the scaling form \[6\]:

$$\beta_L = \beta + \frac{A}{L^\lambda},$$

(10)

where $\beta$ is the asymptotic value of the growth exponent, $\lambda$ determines the correction to the scaling with system size, and $A$ is a constant. The data in Table 2, shown in Fig. 4, for $L = 2^{10} - 2^{17}$ yields $A = -0.530 \pm 0.128$, $\lambda = 0.324 \pm 0.043$, and

$$\beta = 0.336 \pm 0.004.$$ (11)

The data for the largest lattices in Table 2 were excluded from the fitting because of insufficient accuracy, but the best fit still lies within their error bars.

4.4. The growth time

In measuring the growth times $t_g$ in Table 2, we have expanded the criteria suggested by Reis in \[6\] by using floating “beginning” and “end” points for each lattice size and imposing a maximum-time criterion. Figure 5 shows a log-log plot of $t_g$ against $L$ with a straight-line fit of the data points from $L = 2^{16}$ to $L = 2^{20}$. The significance of this graph is that only when its slope, which we call the “growth-time exponent” and denote by $\gamma$, reaches unity can we say with confidence that we have reached the asymptotic regime. The power-law growth regime for a system of size $L$ is influenced by two factors. (i) The transient regime, during which the system first follows random deposition, before the BD rules determine the growth characteristics. This is largely $L$-independent. (ii) The approach to the saturation regime, which corresponds to a deviation from power-law behaviour of the surface width. This is strongly $L$-dependent.

For small system sizes, the transient and saturation regimes are sufficiently close together that the growth exponent deviates significantly from the true asymptotic BD value. In effect, the system never enters a fully-developed BD growth regime. But, as $L$ increases, the time between the transient and saturation regimes increases and eventually these are sufficiently separated that true BD behaviour can develop. It is for these values of $L$ that we observe the slope of unity in Fig. 5.

![Figure 5.](image-url) (Color online) Log-log plot of $t_g$ against $L$ for the data in Table 2. The growth time exponent $\gamma = 1.002 \pm 0.004$ obtained from the slope of a linear fit to the data points from $L = 2^{16} - 2^{20}$ (red dots) approaches unity very closely indicating that the system has entered the asymptotic regime.
5. Conclusion
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 roughness and growth 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 number 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 properties, this is likely an intrinsic property of BD.

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 behaviour persists for higher-dimensional substrates, but we have not yet determined the rate of convergence. This presents a significant computational obstacle for determining the exponents of BD and in establishing the precise relation to the KPZ equation. In this regard, Fig. 5 is vital because it indicates the whether the system has entered the asymptotic regime. This will be taken up in a future publication.

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