Universality of 2+1 dimensional RSOS models

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Extensive dynamical simulations of Restricted Solid on Solid models in $D = 2+1$ dimensions have been done using parallel multisurface algorithms implemented on graphics cards. Numerical evidence is presented that these models exhibit Kardar–Parisi–Zhang surface growth scaling, irrespective of the step heights $N$. We show that by increasing $N$ the corrections to scaling increase, thus smaller step sized models describe better the asymptotic, long wave scaling behavior.

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I. INTRODUCTION

The Kardar–Parisi–Zhang (KPZ) equation \cite{1} describes the evolution of a fundamental, non-equilibrium surface growth model by a Langevin equation

$$\partial_t h(x, t) = \sigma \nabla^2 h(x, t) + \lambda (\nabla h(x, t))^2 + \eta(x, t). \quad (1)$$

The scalar field $h(x, t)$ is the height, progressing in the $D$ dimensional space relative to its mean position, that moves linearly with time $t$. A smoothing surface tension is represented by the coefficient $\sigma$, which competes a curvature-driven propagation, described by the nonlinear coefficient $\lambda$ and a zero-average Gaussian stochastic noise. This noise field exhibits the variance $\langle \eta(x, t)\eta(x', t') \rangle = 2T\delta^D (x - x')(t- t')$, with an amplitude, related to the temperature in the equilibrium system, and $\langle \rangle$ denotes a distribution average. Besides describing the dynamics of simple growth processes \cite{5} KPZ was inspired in part by the stochastic Burgers equation \cite{2} and is applicable for randomly stirred fluids \cite{3}, for directed polymers in random media \cite{4} for dissipative transport \cite{6} 7] and for the magnetic flux lines in superconductors \cite{8}.

Discretized versions have been studied a lot in the past decades \cite{9, 11}. The morphology of a surface of linear size $L$ can be described by the squared interface width

$$W^2(L, t) = \frac{1}{L^2} \sum_{i,j}^L h_{i,j}^2(t) - \left( \frac{1}{L} \sum_{i,j}^L h_{i,j}(t) \right)^2. \quad (2)$$

In the absence of any characteristic length simple growth processes are expected to be scale-invariant

$$W(L, t) \propto L^\alpha f(t/L^z), \quad (3)$$

with the universal scaling function $f(u)$

$$f(u) \propto \begin{cases} u^\beta & \text{if } u \ll 1, \\ \text{const.} & \text{if } u \gg 1 \\ \end{cases} \quad (4)$$

Here $\alpha$ is the roughness exponent in the stationary regime, when the correlation length has exceeded $L$ and $\beta$ is the growth exponent, describing the intermediate time behavior. The dynamical exponent $z$ can be expressed as the ratio of the growth exponents

$$z = \alpha/\beta \quad (5)$$

and due to the Galilean invariance the $\alpha + z = 2$ relation holds as well.

While in $D = 1+1$ exact solutions are known, due to the Galilean symmetry \cite{12} and an incidental fluctuation-dissipation symmetry \cite{13}, in higher dimensions KPZ has been investigated by various analytical \cite{13} and numerical methods \cite{14} 22], still debated issues remain. For example, there is a controversy on the surface growth exponents of the $D = 2+1$ KPZ, obtained by recent simulations \cite{2} 24, 29] and a field theoretical study \cite{25}. Assuming that the height correlations do not exhibit multi-scaling and satisfy an operator product expansion Ref. \cite{25} concluded that growth exponents are rational numbers in two and three dimensions \cite{25}. This was in accordance with some earlier Restricted Solid-on-Solid (RSOS) model simulation results \cite{26} 27]. Recent high precision simulations \cite{23} 24, 28, 30] all excluded this and concluded $\alpha = 0.393(4)$ \cite{23} 24, 30] and $\beta = 0.2414(15)$ \cite{23}. RSOS models are defined by deposition at random sites if the local height difference satisfies

$$|h(x, t) - h(x', t)| \leq N. \quad (6)$$

Very recently Kim \cite{31} investigated RSOS models with maximum step sizes $N = 1, 2, \ldots, 7$. As he increased $N$ the
roughness exponent \( \alpha \) seemed to converge to 4/10 and the growth exponent \( \beta \) to 1/4 in agreement with \cite{25,27}. This issue is important, because one may speculate that discretized simulations cannot describe the local singularities of continuum models, i.e., finite slopes may cause corrections, responsible for the longstanding debate between field theory and discrete model simulations.

In this paper we show that the converse is true. By performing very careful corrections-to-scaling analysis on the model of Ref. \cite{31} we show that even in case of \( N > 1 \) the rational numbers of \cite{25–27} can be excluded in the \( L \to \infty \) limit. Local slopes analysis shows, that the \( N = 1 \) case has the smallest corrections and describes the KPZ universality scaling the best. For \( N > 1 \) corrections corresponding shorter wavelengths are introduced. Our findings are in full agreement with the scaling results obtained for ballistic growth models \cite{24,32,33}.

II. MODELS AND SIMULATION ALGORITHMS

In order to enable long time surface growth simulations of large systems, a multisurface-like parallel implementation of the RSOS model has been implemented for graphics processing units (GPUs). Two parallelization approaches have been combined as follows:

Since GPUs feature a number of vector processors, multiples of 128 realizations of the model were simulated simultaneously. This creates a data-parallel workload, which can straightforwardly be vectorized. Each single instruction multiple thread (SIMT) unit of the GPU updates 128 realizations, in which the sequence of randomly selected coordinates for update is the same. This correlation was broken by updating only half of the selected lattice sites in each attempt. If more realizations were simulated, different sets of 128 realizations evolved completely independently.

In order to handle large systems effectively a domain decomposition (DD) was also used to distribute the work of realizations among multiple SIMT elements. A double-tiling scheme was applied by splitting up the simulation cells into tiles, spitted further into two sub-tiles along each spatial direction \cite{34}. In the present two-dimensional problem this yields \( 2^d = 4 \) sets of sub-tiles, each of which can be updated by multiple independent workers. After each lattice sweep the origin of the DD was moved randomly to eliminate correlations. Implementation details will be published elsewhere \cite{35}.

Roughening of \( d + 1 \)-dimensional RSOS surfaces was studied for restriction parameters \( N = 1, 3, 5, 7 \), by starting from flat initial conditions. To obtain estimates for the exponent \( \beta \), the growth of surfaces was followed up to \( t = 10^5 \) Monte-Carlo steps (MCS), which is well before the correlation length approaches the system sizes: \( L = 4096, 8192 \) and 9605 studied here (throughout this paper the time is measured in MCS). The largest system size was bounded by memory constraints, filling up 12 GB of the NVIDIA K40 GPU, and leaving some memory for the random number generator (RNG) states. The results were averaged over \( n = 768, 128 \) and 128 realizations, respectively, where the latter two correspond to only one multisurface run.

The exponent \( \alpha \) was determined by a finite-size scaling analysis of the saturation roughness of system sizes between \( L = 64 \) and \( L = 512 \). To keep the noise amplitude constant we used domain sizes of \( 8 \times 8 \) lattice sites.

We determined the interface width by averaging over \( W(L, t) \) for times \( t \geq t_{\text{start}} \) and for all samples. We checked whether the averaged values belong to the steady state: \( t > t_{\text{steady,} \alpha} \) by varying \( t_{\text{start}} \), the onset times of the measurements. We estimated \( t_{\text{steady,} \alpha} \) via the relation

\[
\alpha_N \cdot L^\alpha = b_N \cdot t_{\text{steady,} \alpha}^\beta,
\]

using the parameters \( a_N \) and \( b_N \), deduced from fitting in small systems.

In order to estimate the asymptotic values of \( \alpha \) and \( \beta \) for \( L \to \infty \) and \( t \to \infty \), respectively, a local slope analysis of the scaling laws was performed \cite{36}. We calculated the effective exponents

\[
\alpha_{\text{eff}} \left( \frac{L - L/2}{2} \right) = \frac{\ln W(L, t \to \infty) - \ln W(L/2, t \to \infty)}{\ln(L) - \ln(L/2)}
\]

(8)

\[
\beta_{\text{eff}} \left( \frac{t_i - t_{i/2}}{2} \right) = \frac{\ln W(L \to \infty, t_i) - \ln W(L \to \infty, t_{i/2})}{\ln(t_i) - \ln(t_{i/2})}
\]

(9)

In our studies the simulation time between two measurements is increased exponentially

\[
t_{i+1} = (t_i + 10)e^m,
\]

using \( m = 0.01 \) and \( t_0 = 0 \), while statistical uncertainties are provided as \( 1\sigma \)-standard errors, defined as

\[
\Delta_{1\sigma} x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}/(N - 1).
\]

III. SURFACE GROWTH RESULTS

A. The Growth Regime

The growth of the surface roughness follows apparently the same, clear, power-law for all considered \( N \) (Fig. 1 top). The local slope plots (Fig. 1 down), using (9), show an effective growth exponent \( \beta_{\text{eff}} \approx 0.25 \) for \( N = 5, 7 \) for \( t \leq 1000 \text{MCS} \) \((t^{-1/4} \approx 0.18)\), in agreement with Kim’s results \cite{31}. Later, the effective growth exponent decreases for all \( N > 1 \), followed over two orders of magnitude in time \cite{11}.

Expecting independence of \( \beta \) from \( N \), it follows that the asymptotic estimates \( \beta_N \) should be the same. By assuming power-law corrections to the asymptotic scaling \( W(L \to \infty, t) \propto t^\beta (1 + t^{-x}) \), we obtained a minimal variance of the \( \beta_{N>1} \) estimates in case of \( x \approx 0.25 \). Therefore, we plotted our \( \beta_{\text{eff}} \) results on the \( 1/\sqrt{t} \) scale, which
TABLE I: Extrapolated $\beta$ results for different $N$. Figures in the parentheses for $N = 1$ are fit, while for $N > 1$ case is 1σ error estimates.

| $L$  | $\beta_1$          | $\beta_{N>1}$          |
|------|--------------------|------------------------|
| 4096 | 0.2412(1) 0.2418(1) 0.2415(1) | 0.2404(3) 0.2405(3) 0.2410(3) |
| 8192 |                    |                        |
| 9605 |                    |                        |

makes the tails of the curves straight in the $N \to \infty$ limit. Logarithmic corrections to scaling were also tested, but they did not improve the extrapolations.

Table II lists the obtained estimates for $\beta$ for the considered system sizes. Results for different $N > 1$ are practically identical and are thus averaged to give a common value. The case $N = 1$ is listed separately, due to the different corrections to scaling. For $N = 1$, $\beta_{\text{eff}}$ can be best extrapolated by a power-law fit with $x = 0.90(2)$. This is in a good agreement with the results of [37], where $x \simeq 0.96 \simeq 4\beta$ is reported. The estimates show no clear dependence on system size, thus it can be safely assumed that all simulations are well within the scaling regime and do not suffer from finite-size effects. All results are within the margin of error of the octahedron model $\beta = 0.2415(15)$ [28]. Most notably this is also the case for the estimates for $N > 1$. Overall, the present data support $\beta = 0.241(1)$.

Since the curves in Fig. 1 correspond to the same $L$ and sample size $n$, one can observe that the signal-to-noise ratio ($S/N$), the ratio between the interface width and the sample variance, increases with $N$. For $N = 7$ this is higher by a factor of $\sim 3.6$, while for $N = 3$ the $S/N$ is about $\sim 2.5$ bigger than that of the $N = 1$ result. Presumably, the decrease of relative noise level is the consequence of a kind of self-averaging, since systems with larger allowed $N$ accommodate more surface information than smaller ones. It is tempting to exploit this property by choosing larger height differences in the simulations, even if this can be implemented less efficiently. However, as one can observe in Fig. 1 effective scaling exponents for $N > 1$ suffer from stronger corrections than the $N = 1$ case. Furthermore, our data suggest a possible oscillating convergence of $\beta_{\text{eff}}$ for $N > 1$ as in case of Ref. [24].

**B. The Steady State**

Direct fitting of the finite size scaling form

$$W_{\text{sat}}(L) \sim L^\alpha,$$

for $32 \leq L \leq 512$ and $t_{\text{start}} = 50t_{\text{steady}}$ yields the following estimates

$$\alpha_{\text{fit}} = \begin{cases} 
0.392(1) & N=1 \\
0.401(2) & N=3 \\
0.402(2) & N=5 \\
0.402(2) & N=7
\end{cases}$$

for comparison, Kim’s results [31] are shown in the second column. When we decrease $t_{\text{start}}$ our values decrease slightly, but fall inside the error margins if $t_{\text{start}} \geq 2t_{\text{steady}}$. So, direct fits match perfectly those of [31], obtained by sequential Monte Carlo updates.

However, if the $L = 32$ data are excluded, our estimates become significantly lower, warning for strong corrections to scaling. This can also be seen with the help of the effective exponents in Fig. 2 calculated by [3]. There is a clear tendency for $\alpha_{\text{eff}}$ to decrease as we increase the system size for the $N > 1$ cases. The approach to $L \to \infty$ is nonlinear, but the number of points is insufficient for power law (PL) extrapolations to produce consistent estimates. We plotted the $\alpha_{\text{eff}}(L)$ results on the $1/\sqrt{L}$ scale, resulting in points that can be settled on straight lines. Linear extrapolation to asymptotically large sizes yields:

$$\alpha = \begin{cases} 
0.391(1) & N = 1 \\
0.386(1) & N > 1
\end{cases}$$

Corrections to finite-size scaling [11] in case of $N = 1$ are small, explaining the good agreement between local slope
analysis and the direct fit. The slight difference between the $N = 1$ and $N > 1$ results may be attributed to the fact that our data points are not deeply enough from the steady state. This might also explain the disagreement with the results of a recent study [22], which reported $\alpha = 0.3869(4)$ for $N = 1$. There is a further uncertainty of the extrapolation to $L \to \infty$, which is not accounted for by the fit errors. With the assumption of an intrinsic width: $W^2 = 0.2$ [32], the local slopes analysis shows stronger corrections to scaling, therefore we did not apply this in our study.

The observation of stronger corrections for larger $N$’s is consistent with a recent analysis of the ballistic deposition Model (BD). [24] This study found that corrections to scaling, for both $\alpha$ and $\beta$, are reduced, when the BD surface is smoothened by binning of the surface positions before analysis, thereby decreasing the height differences between neighboring sites. Binning of the surface did not change the universal behavior, it only decreased non-universal corrections. The corrections produced even an oscillatory approach to the asymptotic values of the exponents. This can explain why our simple extrapolations of $\alpha_{\text{eff}}$ (Fig. 2) and $\beta_{\text{eff}}$ (Fig. 1) for $N > 1$ undershoot those of $N = 1$.

All of our estimates up to $N \leq 7$, obtained by the local slope analysis, are in the range $\alpha = 0.390(4)$, which clearly excludes $\alpha = 2/5$. Plugging our $\alpha$ and $\beta$ results into the scaling relation [3] we get the dynamical exponent estimates $z_{N=1} = 1.61(2)$ and $z_{N>1} = 1.60(2)$, respectively. The scaling law following from the Galilean invariance is satisfied with these exponents both for $N = 1$: $\alpha + z = 2.01(2)$ and $N > 1$: $\alpha + z = 1.99(2)$ within error margins.

We have also tested the scaling form [3] numerically by using our $\alpha$ and $\beta$ values. As Fig. 3 shows good data collapses can be obtained for $N > 1$ and even a perfectly looking one for $N = 1$. For $N > 1$ in the growth regime a perfect one can also be achieved assuming the values suggested by Kim and Kosterlitz [25] (Fig. 3 top). This can be understood by taking into account the corrections to scaling we explored above. Effective exponents for early times and small systems agree with the conjecture by [26] and indeed the most strongly outlying curves in Fig. 3 top, correspond to smaller systems.

We also calculated some standard measures, the skewness

$$ S = \frac{\langle (\Delta h)^3 \rangle}{\langle (\Delta h)^2 \rangle^{3/2}} $$

(12)

and the kurtosis

$$ Q = \frac{\langle (\Delta h)^4 \rangle}{\langle (\Delta h)^2 \rangle^2} - 3 $$

(13)

of our width-distributions in the steady state. The obtained values show no significant dependence on $N$, our best results are $S = 1.70(1)$ and $Q = 5.38(4)$, in good agreement with those of [22].
The differences among the results of the considered DD configurations were not significant in the data collapses, nor in the finite-size scaling fits. The most sensitive quantity proved to be the effective roughness exponent, shown in Fig. 4. Sample sizes of this test were not significant, although small systematic errors might be present.

IV. CONCLUSIONS

Extensive numerical simulations have been performed for $2 + 1$ dimensional RSOS models with variable height difference restrictions. Careful correction to scaling analysis has provided numerical evidence, that the universal surface growth exponents agree with the most precise values known for the $2 + 1$ dimensional KPZ class. These estimates: $\alpha = 0.390(4)$ and $\beta = 0.2415(3)$ exclude the rational values $\alpha = 4/10$ and $\beta = 1/4$, conjectured by [25–27,31]. Our results support the generalized KPZ ansatz, which takes finite time corrections into account and predicts exponents $x$ that are multiples of $\beta$ [37]. We found $x = 0.90(2)$ for $N = 1$ and $x \approx 0.25$ for $N > 1$. We have shown that by increasing the local height differences we obtain better $S/N$ in the simulations, but stronger corrections to scaling, which can confuse numerical analysis based on simple power-law fitting. Therefore, smaller step sized models, like the octahedron model [24] describe better the asymptotic, long wave scaling behavior of the KPZ universality class. Our conclusions for scaling-corrections are in agreement with those, obtained for ballistic growth models [24,32].
vided estimates for the skewness $S = 1.70(1)$ and the kurtosis $Q = 5.38(4)$ of the steady state surface width distributions. Our simulations have been performed using multisurface GPU SIMT algorithms with origin moving domain decomposition. The results have been justified by varying the tile sizes. A sustained performance of $\simeq 1.1 \times 10^{10}$ deposition attempts per second could be achieved running on a single NVIDIA GTX Titan Black GPU. This opens up the possibility for precise RSOS simulations in higher dimensions.

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