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Multisurface coding simulations of the restricted solid-on-solid model in four dimensions

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We study the restricted solid-on-solid model for surface growth in spatial dimension $d = 4$ by means of a *multisurface coding* technique that allows us to analyze samples of size up to 256^4 in the steady-state regime. For such large systems we are able to achieve a controlled asymptotic regime where the typical scale of the fluctuations are larger than the lattice spacing used in the simulations. A careful finite-size scaling analysis of the critical exponents clearly indicate that $d = 4$ is not the upper critical dimension of the model.

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The Kardar-Parisi-Zhang (KPZ) equation [1] is possibly the simplest, most studied, and yet not fully understood model for out-of-equilibrium surface growth. The equation describes the time evolution of the height $h(\mathbf{r},t)$ of an interface above a d-dimensional substrate

$$\partial_t h(\mathbf{r},t) = \nu\vec{\nabla}^2 h(\mathbf{r},t) + \frac{\lambda}{2}|\vec{\nabla}h(\mathbf{r},t)|^2 + \eta(\mathbf{r},t), \qquad (1)$$

where ν is the diffusion coefficient, λ is the strength of the nonlinear growth rate term which is responsible for the $h \to -h$ symmetry breaking with respect to the growing direction, and $\eta(\mathbf{r},t)$ is a Gaussian white noise of amplitude D,

$$\langle\eta\rangle = 0, \quad \langle\eta(\mathbf{r},t)\eta(\mathbf{r}',t')\rangle = 2D\delta^d(\mathbf{r}-\mathbf{r}')\delta(t-t'). \qquad (2)$$

The KPZ equation describes many relevant growth processes, such as the Eden model, ballistic deposition, and interface growth in disordered medium. It is also related to many other physical phenomena apparently unrelated to surface growth, such as Burgers turbulence, dynamics directed polymers in random media, and dissipative transport in the driven-diffusion equation [2].

The scaling properties of the height's fluctuations $w_2(L,t) = \langle h^2(\mathbf{r},t)\rangle_{\mathbf{r}} - \langle h(\mathbf{r},t)\rangle_{\mathbf{r}}^2$ (with the notation $\langle\ldots\rangle_{\mathbf{r}}$ we indicate a spatial average over a macroscopic hypercubic box of linear size L over the d-dimensional substrate) characterize the universality class of the model. More precisely, for a system of size L, $w_2(L,t) \sim L^{2\chi} f(t/L^z)$, where the scaling function is such that $f(x) \to$ const for $x \to \infty$ and $f(x) \sim x^{2\chi/z}$ for $x \to 0$. The peculiar behavior of f imply that $w_2(L,t) \sim L^{2\chi}$ for $t \gg L^z$ and $w_2(L,t) \sim t^{2\chi/z}$ for $t \ll L^z$. Due to an infinitesimal tilt symmetry of Eq. (1) ($h \to h + \mathbf{r}\cdot\boldsymbol{\epsilon}$, $\mathbf{r} \to \mathbf{r} - \lambda t\boldsymbol{\epsilon}$), the two critical exponents are related by the scaling relation $\chi + z = 2$, which is believed to be valid at any dimension d [2].

A complete understanding of Eq. (1), and in particular the determination of the two critical exponents χ, z for any spatial dimension $d > 1$ (at $d = 1$ a fluctuation-dissipation theorem leads to the exact result $\chi = 1/2$, $z = 3/2$), turns out to be extremely difficult for two main reasons: (i) we are dealing with an intrinsically out-of-equilibrium phenomenon where the standard equilibrium toolbox must be used with care and (ii) perturbative renormalization schemes are not adequate for describing the strong coupling regime (i.e., where the parameter λ is relevant).

The existence of an upper critical dimension d_u, i.e., the substrate dimensionality d above which the fluctuation of the model become irrelevant ($\chi = 0$), is one of the most controversial unsolved theoretical issues related with Eq. (1). The determination of d_u would be a most relevant achievement since, as customary in equilibrium critical phenomena, its knowledge constitutes the first step for a controlled perturbative expansion around it. The quest for d_u has been around for more than 20 years [3–18] and the different predictions range from $d_u \approx 2.8$ to $d_u = \infty$. Analytical estimates using the mode-coupling theory yield exact results in $d = 1$ [19]. Their extension to higher dimensions hints for a $d_u = 4$ under different self-consistency schemes [5–9]. The same value for d_u is also supported by different field-theoretic approaches [3,10,11,14,15], whereas in Ref. [16] a nonperturbative renormalization group technique is proposed, yielding a finite (although very small compared with numerical simulations) scaling coefficient χ in $d = 4$.

At odds with what is predicted by the previously mentioned field-theoretic approaches, both direct numerical integration of KPZ equation [20] and simulation of systems belonging to the KPZ universality class [13,17,21–25] indicate that $d_u > 4$, while the real-space renormalization group approach [18] predicts $d_u = \infty$.

Such a long-standing controversy is the consequence of the difficulties inherent to both analytical and numerical approaches. Most of the assumptions made on the functional structure of the sought solution in the different field-theoretic analysis, as well as the approximations made in the mode-coupling theories are, in general, not completely under control. On the numerical side, the most severe problem is due to the fact that simulations in high spatial dimensions $d \geqslant 4$ are computationally very heavy, and the systems under analysis must be limited in size. As a consequence, the different fitting procedures must deal with controlled finite-size scaling procedures to yield reliable estimates of the critical exponents. Under this perspective, particularly relevant is the observation that, for lattice models in the KPZ universality class, a controlled asymptotic regime is achieved only when the typical scale of the fluctuations is larger than the lattice spacing used in the simulations or, more precisely, for $w_2 > 1$ [9]. The former

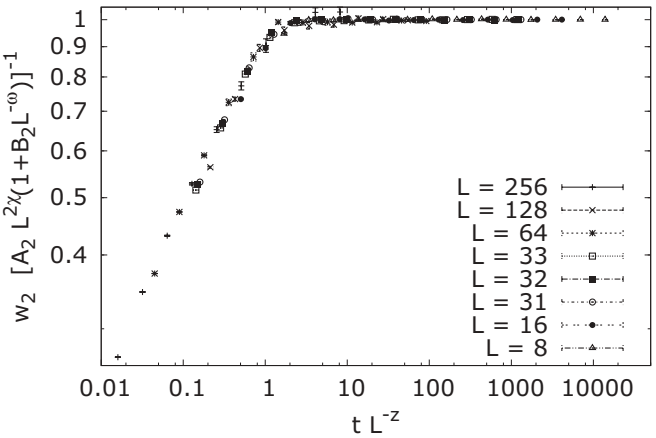

FIG. 1. Scaling plot of the rescaled second moment $w_2/[A_2L^{2\chi}(1+B_2L^{-\omega})]$ vs. the rescaled time t/L^z.

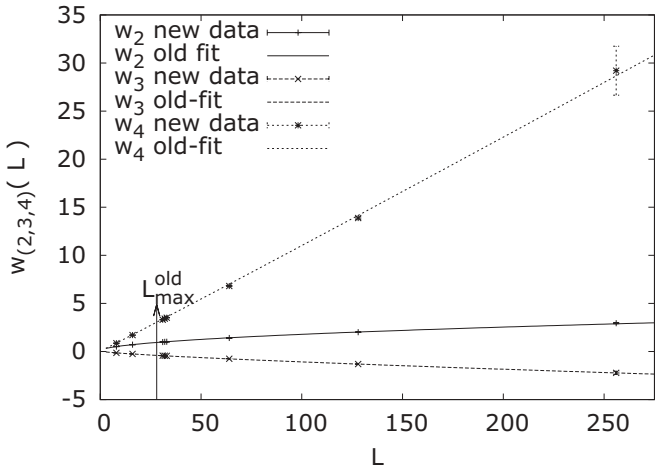

FIG. 2. The quantities w_2, w_3, w_4 are displayed as a function of L. Dots with error bars are values obtained by simulations, while solid lines are the eight-parameter best-fit reported in Ref. [13]. The vertical arrow arrow at $L = 28$ represents the largest size simulated in Ref. [13].

inequality is very stringent from the computational point of view since it requires very large lattices to be fulfilled: The estimates presented in Refs. [13,23] suggest indeed that for the four-dimensional restricted solid-on-solid (RSOS) model, to which this Rapid Communication is addressed, the $w_2 > 1$ inequality starts being verified for lattice size larger than $L \approx 32$, whereas the larger system size analyzed in the steady-state regime is $L = 128$ [23] that, to the best of our knowledge, remains the larger system in four dimensions simulated so far.

To settle the controversy, at least in the four-dimensional RSOS model case, we decided to analyze samples of unprecedented size: We have been able investigate the steady-state scaling regime $t \gg L^z$ for lattice size volumes up to $V = 128^4 = 268\,435\,456$ sites, a factor 16 off the largest simulation known in the literature [23] in the steady-state regime. We can also study the dynamic scaling regime of lattices of $V = 256^4 = 4\,294\,967\,296$ sites, but for such a large size we have been able to investigate the asymptotic scaling regime for just three samples, due to limitations in our computing facility (most of the data for $L = 256$ are at not too large t and they have been used only in Figs. 1 and 2; they appear only in the region $t/L^z < 8$).

The RSOS can be simulated in the following way: At any time t, we randomly select a site i on the d-dimensional lattice and we let the surface height h_i at that point to grow of a unit $h_i(t+1) = h_i(t) + 1$ only if $\max_{j\in\partial i} |h_i(t) - h_j(t)| \leqslant 1$, being ∂_i the set of eight nearest neighbors of i in $d = 4$ (note that we will assume periodic boundary conditions).

We simulated RSOS growth using two different algorithms based on a very efficient *multispin coding* technique [26] originally developed for a disordered spin system and later generalized to deal with the RSOS model [13] as follows:

(i) *Multisurface (MS) coding:* We can simulate, with basically the same cost of one single surface simulation, N_b copies of the system, N_b being the number of bits in the computer world (usually 32, 64, 128, and 256). We transform the basic operations (like summing spins for computing the effective force) into Boolean operations, and we exploited the fact that when, for instance, the computer is calculating an AND logical bit, it is indeed doing that operation N_b times at once, i.e., for all the bits of the world. Unfortunately, computational efficacy of this method is counterbalanced by the memory load, making it unpractical for analyzing samples of linear size larger than $L = 64$, at least on the computers we have access to.

(ii) *Multiattice-site (ML) coding*: For a sample of linear size $L = 128,256$ we have developed a new multispin coding representation in which a single surface at time is simulated, but we lump together the N_b height-difference local variable in a single computer word of N_b bits. We will refer to this second method as the multiple-lattice-site (ML) algorithm (see Table I). In this algorithm, in the first half step we update the even spins (i.e., the spins σ_i where $i_x + i_y + i_z + i_t$ is even), applying the standard RSOS procedure with probability $1/2$ to each spin (with probability $1/2$ the spin is not updated), and, in the second half step, we apply the algorithm to odd spins. Some programming care must be used with periodic boundary conditions: In the simplest version we have used, L must be an even multiple of N_b. Moreover, it is crucial to use a good random number generator, where *all* the bits are random.

We simulate four-dimensional lattices of volume $V = L^4$ for lattices of linear size $L = 8,16,31,32,33,64,128,256$. For the two largest lattices ($L = 64,128,256$), we run the ML

TABLE I. The lattice linear size L, the number of Monte Carlo sweeps (full lattice update), the number of samples, the simulation type (MS = multisurface coding, ML = multilattice coding), and the overall computational time in hours.

L	Sweeps	Samples	Type	Time (h)
8	524 000	1024	MS	4
16	524 000	1024	MS	6
31	524 000	1024	MS	121
32	524 000	1024	MS	139
33	524 000	1024	MS	158
64	131 000	512	MS	5376
128	512 000	64	ML	7680
256	130 000	64	ML	504

TABLE II. The best fit values together with their statistical error of the parameters defined in Eq. (4). The first row refers to the actual data presented in this work and the second is taken from Ref. [13]. The value for χ is in good agreement with the result $\chi = 0.245(5)$ reported in Ref. [23] for the directed 4-mer diffusion model.

	χ	ω	A_2	B_2	A_3	B_3	A_4	B_4
New	0.2537(8)	1.11(9)	0.171(1)	0.37(6)	0.0319(3)	−1.0(2)	0.100(1)	0.38(8)
Old	0.255(3)	0.98(9)	0.170(1)	0.37(3)	0.0321(2)	−0.7(1)	0.100(1)	0.46(4)

algorithm, while for the rest we run the MS algorithm. We decided to consider $L = 31,33$ for checking that there are no periodicity issues with the random number generator. A summary of our simulations is provided in Table I.

The simulations aim at achieving a fair sampling of the asymptotic regime. To do so, at any time t and for each sample (both in ML and MS type of simulation) we evaluate the first three connected moments $w_n(L,t) = \sum_{i=1}^{V}(h_i(t) - \langle h(t)\rangle)^n / V$, where $\langle h(t)\rangle = \sum_{i=1}^{V} h_i(t)/V$ and $n = 2,3,4$. We thus define our asymptotic (in time) estimate as

$$w_n(L) = \frac{1}{T_0 - T_1 + 1}\sum_{t=T_1}^{T_0} w_n(L,t). \tag{3}$$

We are careful to choose both T_0, and $T_1 - T_0$ large enough to guarantee (i) convergence to the asymptotic regime, i.e., that $T_1 \gg L^z$, and (ii) a large-enough sampling of statistically uncorrelated measures of $w_n(L,t)$. In practice, we consider consecutive measuring windows of length $64,128,\ldots,T_1,T_0$, so T_0 is the last measure in the simulation and $T_1 = T_0/2$. This choice is very conservative, since eventually we use just the second half of the simulation, but, at the same time, it allows us to check with very high reliability whether we have reached the asymptotic state. A quick look at Fig. 1 shows the results of having chosen for $L = 128$ a $T_0 \gg L^z$, at least of a factor 100 off, whereas for $L = 256$, due to the computational cost, it is only a factor 10 off. We are now ready to determine the critical exponents of the asymptotic behavior of w_n, which scales as $L^{n\chi}$ at the leading order, by fitting simultaneously the following moments [13,27]:

$$\begin{aligned} w_2 &= A_2 L^{2\chi}(1 + B_2 L^{-\omega}),\\ w_3 &= A_3 L^{3\chi}(1 + B_3 L^{-\omega}),\\ w_4 &= A_4 L^{4\chi}(1 + B_4 L^{-\omega}), \end{aligned} \tag{4}$$

where ω is the leading finite-size scaling exponent. The fit involves the simultaneous determination of eight parameters whose best-fit value is reported in the first row of Table II (the fit yields a χ^2 root-mean-square deviation of 2.05). Interestingly, the fit presented in Ref. [13] agrees very well with the new data, as we can clearly appreciate qualitatively in Fig. 2, and more quantitatively by comparing the two rows in Table II. With respect to the $w_2 > 1$ inequality issue, a glance at Fig. 2 shows unambiguously that the scale of the typical fluctuations, for all lattice size larger than $L = 31$, verify the inequality. We do not see any change in the scaling behavior of the three cumulants around the crossover region $L \approx 30$; moreover, the fact that the old fit presented in Ref. [13] (in a regime $w_2 < 1$) agrees so well with our larger lattice size simulation (see again Fig. 2) indicates that the simulations performed for $L \leqslant 28$ were able to capture fairly the asymptotic scaling regime. To see more clearly the finite-size corrections of χ we determined the effective exponent χ_n^{eff} as the discretized logarithmic derivative of Eqs. (4), which in our case reads

$$\chi_n^{\text{eff}}(L) = \frac{\log\left(\frac{w_n(L)}{w_n(L')}\right)}{n\log\left(\frac{L}{L'}\right)}, \tag{5}$$

where $L/L' = 2$ and $n = 1,2,3$. In Fig. 3 we display χ_n^{eff} as a function of L^{-1} (note that we discarded for the sake of clarity the $L = 31,33$ results) for the three cumulants together with the best-fit curves. The fit yields the following results for the critical exponents: $\chi = 0.2532(5)$ and $\omega = 1.14(5)$ (see also Table II). Our estimate for the χ exponent compares very well with the recent result obtained in Ref. [23] for the directed 4-mer diffusion model where a value $\chi = 0.245(5)$ is reported. Recent work has investigated a model of direct polymers in a random medium that should belong to the same universality class [24]. In this model one can define an exponent ζ that, according to the theoretical expectations, should be given as

$$\zeta = \frac{1}{2 - \chi}. \tag{6}$$

Their results (ζ slightly larger than 0.57) are consistent with our prediction $\zeta = 0.5725(2)$.

The numerical technique we have introduced has allowed us to run very precise numerical simulations of the RSOS model in $d = 4$ on unprecedented system size with a limited amount of computational time. Thanks to the accuracy of the simultaneous measurement of the three cumulants, the claim that $d = 4$ is the upper critical dimension for systems in the KPZ universality class has to be rejected. Moreover, the typical

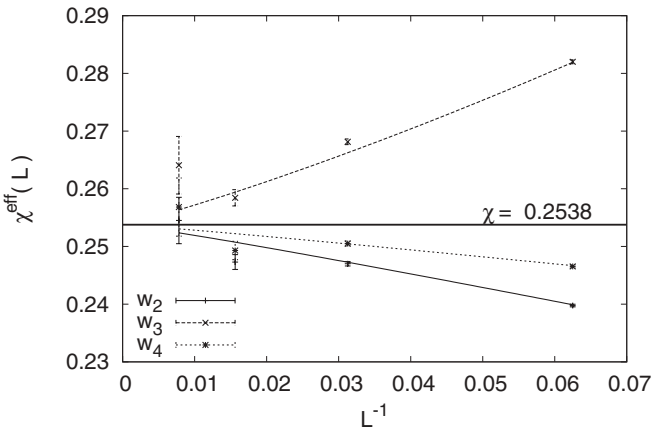

FIG. 3. Local slopes of $w_{2,3,4}$ are displayed as a function of L^{-1}. Dots with error bars are values obtained by simulations, while lines are the eight-parameter best-fit reported in Table II. The solid horizontal line is at $\chi = 0.2538$, i.e., the best-fit prediction for the wandering exponent.

fluctuation's length scale of our simulations on samples of linear size $L = 128$ and $L = 256$ are larger than the lattice spacing, and this is a clear indication that (i) the system reached a controlled scaling regime and (ii) the measured scaling exponents are reliable and not affected by a preasymptotic crossover regime.

There is still a remote possibility that our data are consistent with an upper critical dimension $d_u = 4$ of the KPZ equation if we drop the hypothesis that RSOS in $d = 4$ belongs to the KPZ universality class. However, apart from some work in the past [28], this hypothesis does not seem to have support in the mainstream literature on KPZ.

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