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A Monte Carlo renormalization group study of driven interface dynamics

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Abstract. We have extended the Monte Carlo renormalization group technique to study the dynamics of driven interface systems. The method allows systematic elimination of irrelevant scaling fields and thus helps in extracting the asymptotic scaling behaviour. In particular, it can be applied to determine scaling exponents from a matching criteria. We have applied this method to interfaces evolving according to the Kardar, Parisi and Zhang equation.

The dynamic evolution of spatial patterns is one of the most exciting areas of nonlinear phenomenology. A particular aspect of this general problem involves the growth of thin interfaces in far-from-equilibrium conditions. Well known examples include directional solidification in binary alloy systems [1], dendritic growth [2], viscous fingering in Hele–Shaw cell [3], and film growth by vapour deposition [4]. These problems usually involve nonlinear, non-local dynamical equations for the time evolution of the interface shape (for recent reviews, see [5]). Recently, Jasnow and Viñals provided evidence that the transient dynamics in the viscous fingering problem has a self-similar growth regime [6]. They further developed a numerical renormalization group (RG) method to extract the scaling exponents of such a growing interface. In this method, one maps the two phases separated by the interface onto a spin system upon which the usual Wilson-type block-spin transformation is applied [7]. The transverse length scale, i.e. the finger width, is then used to force a match at different times and different blockage. From these matching conditions one obtains the scaling exponent [6–8].

While the method of Jasnow and Viñals is ideal for dynamical systems where a finite wavelength pattern is selected, such as in the viscous fingering problem, there are other situations where there is no such selection and the interface shape is random. In this case a proper matching condition is needed if one is to apply numerical RG. Furthermore, there are cases where the transverse and longitudinal lengths scale differently [9]—special care must be taken in these situations. The purpose of this short article is to present a generalization of the Monte Carlo renormalization group† (MCRG) technique applicable to problems of interface dynamics far from equilibrium. As an illustration we apply the MCRG method to the problem of kinetic roughening of an interface growing under non-equilibrium conditions [11].

† By Monte Carlo renormalization we mean a numerical RG. For a review see [10].

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Perhaps the simplest model for kinetic roughening in driven interface growth is the stochastic nonlinear partial differential equation proposed by Kardar, Parisi and Zhang (KPZ) [12]:

$$\frac{\partial h}{\partial t} = \nu \nabla^2 h + \frac{\lambda}{2}(\nabla h)^2 + \eta. \tag{1}$$

Here $h(\boldsymbol{x}, t)$ is the height of the interface from a reference plane at position $\boldsymbol{x}$ and time t. It is assumed to be a single valued function. The stochastic noise η satisfies Gaussian statistics with a second moment

$$\langle \eta(\boldsymbol{x}, t)\eta(\boldsymbol{x}', t')\rangle = 2D\delta(\boldsymbol{x} - \boldsymbol{x}')\delta(t - t') \tag{2}$$

where the angular brackets denote an ensemble average. D, ν and λ are constants. Consider the behaviour of an interface evolving according to (1). With time, noise causes the interface to roughen and form correlations of the heights on ever larger length scales (see figure 1). The nonlinear term, which has a purely kinetic origin, causes the average position of the interface to move forward in time. The interface therefore never equilibrates, but rather reaches a steady state. In the absence of the nonlinear term, (1) describes the dynamics of equilibrium roughening [13].

While the KPZ equation is an important model for driven surface growth, its importance extends into several other physics problems. For example, it describes the long-time behaviour of a randomly stirred fluid [14], the growth properties of the Eden model (see, for example, [15]), the behaviour of directed polymers in random media [16], and the evolution of flame fronts [17]. This is due to the fact that the KPZ equation is a variant of the ubiquitous noise-driven Burger's equation.

In studying the kinetics of driven interfaces, the universal, long-time, long-wavelength properties of the interfacial width W are of particular interest. The scaling behaviour of W, and that of the associated correlation functions, is given by the scaling exponents χ and z, which determine the scaling of the height and time variables, respectively. Because of the Galilean invariance of the KPZ equation, these exponents obey a scaling relation

$$\chi + z = 2. \tag{3}$$

At early time $t \ll L^z$, the width scales like $W \sim t^\beta f(tL^{-z})$, where $\beta = \chi/z$ and L denotes the linear system size. At late times $t \gg L^\chi$, the width saturates according to $W \sim L^\chi g(tL^{-z})$. Here $g(x)$ and $f(x)$ are scaling functions [9]. Since W is essentially the one-point correlation function, this scaling indicates that the transverse ($\boldsymbol{x}$) and longitudinal (h) lengths scale differently with L.

For substrate dimension $d = 1$ (and spatial dimension $d + 1$), the exponents can be calculated exactly [12]: $\chi = \frac{1}{2}$ and $z = \frac{3}{2}$. These values have been confirmed by many numerical studies. For the more interesting case of $d = 2$, no exact results are known and one is forced to use numerical solutions. However, numerical studies are hampered by large fluctuations and crossover effects. To date, they do not provide a unique answer [18–20]. The numerical difficulty one is faced with at $d = 2$, the critical dimension of the KPZ equation, is actually a common one. For instance, the numerical simulations on the stochastic Sivashinsky equation, the equation which describes certain flame front propagation, is also hampered by similar difficulties [21, 22 (and references therein)].

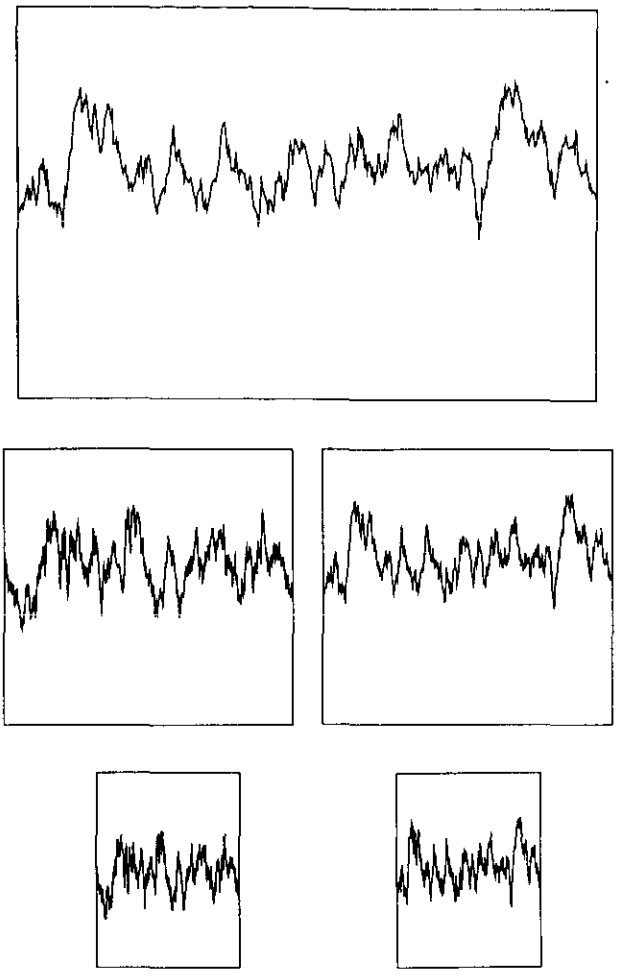

Figure 1. The top interface is for a system of size $L = 4096$ at $t = 400$; the two interfaces on the lower right are the same system at RG stages $m = 1$ and 2. Configurations on the lower left are those for the syste of size $L = 2048$ at $t = 141$, and the same system with one stage of renormalization. Note the similarities between the corresponding sized system.

It is known that MCRG study is useful when the dynamics is controlled by several fixed points; these cause severe crossover effects in most numerical studies. In these situations transient behaviour often obscures the true asymptotic behaviour of the system, particularly when the properties are only accessible through simulations on finite-sized lattices. The RG transformation helps by iterating away irrelevant length scales, driving the system closer towards the fixed point controlling the asymptotic dynamics. Recent successes in the application of MCRG to non-equilibrium systems include studies of the kinetics of domain growth [7], spinodal decomposition [8], the transient dynamics of viscous fingering mentioned previously [6] and a study on aggregation processes [23]. While there is no theoretical proof that the RG transformations used in these works lead to a physical fixed point, the final results derived from the transformations do indicate that the method is correct. In the following, we will thus

be guided by the RG transformations used there.

From figure 1, it is clear that the interface evolving according to (1), after a Wilson-type 'block-spin' transformation (see later), is similar to its earlier state. The system remains approximately invariant under a change of length scales, provided we rescale both the height and time properly. The relationship between the two, combined with the scaling relation (3), determines the value of the exponents.

We first numerically integrated the KPZ equation on a grid to some time t. The transverse coordinate x was then divided into cells of linear size $b = 2$. The height variables $h(x)$ inside each cell was averaged and then rescaled by a factor b^{χ}. This completes a level of RG transformation. We repeat this procedure to get higher levels of the transformation. Figure 1 shows typical results for $d = 1$. For all levels of renormalization m, we measured the interfacial width $W(L^d, m, t) = \sqrt{[\langle (h - \langle h \rangle)^2 \rangle / L^d]}$.

We obtained z through the following matching procedure. In principle, after the irrelevant variables have been iterated away, and the system is close to its strong-coupling fixed point, the probability distributions governing the system remain invariant under further renormalizations. Therefore, any quantity determined after m transformations of the interface of size L^d should be identical to those obtained after $m + 1$ transformations of a $(Lb)^d$ sized system. However, since the time scales in the larger system have been renormalized one more time, the quantities will be at different times t and t'; i.e. $W(L^d, m, t) = W((Lb)^d, m + 1, t')$. This is our matching criterion. The time rescaling factor is then related to z by $t'/t = b^z$. To ensure that the system is close enough to its fixed point, the matching should occur over several values of m. In order for this procedure to work, one must know how to rescale the height variables properly. In other words, we must know χ, whose value is, as yet unknown. We therefore chose many trial values for χ and used the matching condition to get a corresponding z. These values were then used to check whether (3) is obeyed. The pair that satisfied this relation with the smallest error was taken to be the asymptotic result. We refer this procedure as 'predicted matching' since the value of z is predicted from matching.

In $d = 1$, we integrated the KPZ equation using an Euler scheme up to $t = 400$ using a mesh size of $\Delta x = 1.0$ and a time step $\Delta t = 0.01$. The parameters were chosen to be $2D/\Delta t = 1$, $\nu = 1.0$ and $\lambda = 70$. We studied systems of size $L = 4096$ and $L = 2048$. To obtain reasonable statistics we averaged over 100 independent runs for each L. In this case seven different matchings as described earlier were carried out. From this matching procedure, our estimates from matching at different levels of the RG are listed in table 1. Note that the values of χ have essentially converged after three RG levels on the larger system. This gives an average value of $\chi = 0.48$ and $z = 1.52$, with an error of about 5%, in reasonable agreement with the known results.

As a second check, we assumed the time rescaling relationship $t'/t = b^z$ was true explicitly. Thus giving a time t of the 2048 system, the corresponding t' of the 4096 system is computed. If the values used for χ and z were correct, the widths of the two systems at t and t' should be equal—differences between the widths were taken to be due to an incorrect choice of the exponent χ. For each pair of the trial χ and z, the percentage errors between the widths were calculated as function of time t. The value of the exponents for which the error is smallest served as a selection criterion. Note this 'forced matching' procedure assumes a value for z in the beginning. The results of this procedure are listed in table 1. The estimated values of the exponents

Table 1. Roughness exponent χ in one dimension for different levels of RG. System sizes of $L = 2048$ and 4096 are used to do the matching. Other parameters are $\nu = 1.0$, $\lambda = 70$, $2D/\Delta t = 1$, $\Delta t = 0.01$. The first row lists the matching levels of RG on each system. The second row are values of χ from forced matching. The third row are from predicted matching. The values have essentially converged after three RG levels.

0/1	1/2	2/3	3/4	4/5	5/6	6/7
0.476	0.480	0.482	0.482	0.484	0.483	0.481
0.475	0.479	0.480	0.482	0.481	0.482	0.478

are $\chi = 0.48$ and $z = 1.52$, with errors of about 5%. Again, these results are consistent with the known results.

For $d = 2$, the same procedure was repeated. We integrated the KPZ equation up to $t = 160$ using $\Delta t = 0.001$ and $\Delta x = 1.0$. The parameters were chosen to be $2D/\Delta t = 1$, $\nu = 1.0$ and $\lambda = 240$. We simulated systems of size $L^2 = 512^2$ and $L^2 = 256^2$. The results were averaged over 40 and 50 independent runs for the two systems respectively. To make sure that one is well into the asymptotic regime, two test runs were also performed up to $t = 750$ for each of the systems. The two different matching procedures mentioned previously were applied here and the results are listed in table 2. The values of χ have not converged for the five levels of RG possible on these system sizes. The last stage of RG gives $\chi \approx 0.298$ and $z \approx 1.7$, which indicates $\beta \approx 0.17$. The values of β for all stages of RG are smaller than that of [20], and closer to those in [18] and [19]. However, in order to make a conclusive study, larger systems are needed such that more RG iterations can be carried out†.

Table 2. Roughness exponent χ in two dimensions for different levels of RG. Linear system sizes of $L = 256$ and 512 are used to do the matching. Other parameters are $\nu = 1.0$, $\lambda = 240$, $2D/\Delta t = 1$, $\Delta t = 0.001$. The first row lists the matching levels of RG on each system. The second row are values of χ from forced matching. The third row are from predicted matching.

0/1	1/2	2/3	3/4	4/5
0.161	0.230	0.263	0.281	0.298
0.160	0.230	0.263	0.282	0.299

As mentioned previously, the RG transformations help to iterate irrelevant length scale away and reveal the asymptotic behaviour of the dynamics. It also allows us to study the crossover effect known to occur in the KPZ equation [24, 25], in $d = 1$. We used the same parameters as quoted earlier except that the nonlinear coupling constant was smaller, $\lambda = 30$. This value of λ gives quite a wide range in time over which the system crosses over from the trivial fixed point controlling the equilibrium roughening dynamics to the strong coupling fixed point of the KPZ equation [24]. We integrated KPZ equation to $t = 200$ and averaged over 200 independent runs. Fixing the exponent $\chi = 0.5$, the matching procedures described earlier gave values of z at various times. However, at a given time, we expect that higher levels of RG should give values closer to the asymptotic result. In figure 2 the values of z at

† The current study required more than 300 CPU hours on a Cray XMP computer. A comparable study of larger-sized systems in 2+1 dimensions will require at least 20 to 50 times more computer time.

different times are plotted for RG levels of $m = 2, 4, 6$ on the larger system, which is matched with $m = 1, 3, 5$ of the smaller system. We found that higher level matching consistently gives values closer to the asymptotic result $z = 1.5$ at earlier times. This indeed indicates that the RG procedure iterates irrelevant scales away making the system closer to the asymptotic regime. A similar trend was also observed in $d = 2$.

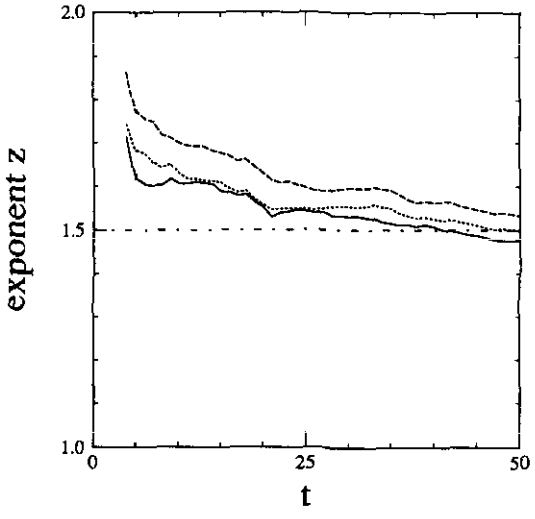

Figure 2. The exponent z in $d = 1$ obtained from the matching procedure at different times, for two systems of sizes $L = 4096$ and $L = 2048$ respectively. Other parameters are $\nu = 1$, $\lambda = 30$, $D/\Delta t = 1$, and $\Delta t = 0.01$. The full curve is for matching of RG levels $m = 6$ with $m = 5$ of the two systems; the dotted curve is for $m = 4$ with $m = 3$; the broken curve is for $m = 2$ with $m = 1$. Note higher levels of RG give values of z closer to the asymptotic result at earlier times.

To conclude, we have extended the MCRG technique to driven interface dynamics, in particular to the KPZ equation. We believe that this method is general and can be readily applied to other systems where dynamic scaling is present.

Acknowledgments

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References

[1] Jackson K A and Hunt J D 1965 *Acta Metall.* **13** 1215
Trivedi R 1987 *Met. Trans.* A **15** 1392
Heslot F and Libchaber A 1985 *Phys. Scr.* T **9** 126
Bachhoefer J and Libchaber A 1987 *Phys. Rev.* B **35** 1392
[2] Huang S C and Glicksman M E 1981 *Acta Metall.* **29** 701; 1981 *Acta Metall.* **29** 717
Dougherty A, Kaplan P D and Gollub J P 1987 *Phys. Rev. Lett.* **58** 1652
[3] Saffman P G and Taylor G I 1958 *Proc. R. Soc.* A **245** 312
[4] Bales G S, Redfield A C and Zangwill A 1989 *Phys. Rev. Lett.* **62** 776

[5] Langer J S 1986 *Chance and Matter, (Proc. Les Houches Summer School Session 46)* ed J Souletie, J Vannimenus and R Stora (Amsterdam: North-Holland)
Kessler D, Koplik J and Levine H 1988 *Adv. Phys.* **37** 255
[6] Jasnow D and Viñals J 1990 *Phys. Rev.* A **41** 6910
[7] Viñals J, Grant M, San Miguel M, Gunton J D and Gawlinski E T 1985 *Phys. Rev. Lett.* **54** 1264
Kumar S, Viñals J and Gunton J D 1986 *Phys. Rev.* B **34** 1908
[8] Roland C and Grant M 1988 *Phys. Rev. Lett.* **60** 2657
Roland C and Grant M 1989 *Phys. Rev.* B **39** 11 971
[9] Family F and Vicsek T 1985 *J. Phys. A: Math. Gen.* **18** L75
[10] Swendsen R H 1982 *Real-Space Renormalization* ed T W Burkhardt and J M J van Leeuwen (New York: Springer) p 57
[11] Krug J and Spohn H 1991 *Solids Far From Equilibrium: Growth, Morphology and Defects* ed C Gordèche (Cambridge: Cambridge University Press)
[12] Kardar M, Parisi G and Zhang Y C 1986 *Phys. Rev. Lett.* **56** 889
[13] Grossmann B, Guo H and Grant M 1991 *Phys. Rev.* A **43** 1727
[14] Forester D, Nelson D and Stephan M 1977 *Phys. Rev.* A **16** 732
[15] Eden M 1961 *Proc. Fourth Berkeley Symp. Mathematics, Statistics and Probability* vol 4, ed F Neyman (Berkely, CA: University of California Press) p 223
[16] Kardar M and Zhang Y C 1987 *Phys. Rev. Lett.* **58** 2087
[17] Medina E, Hwa T, Zhang M and Zhang Y C 1989 *Phys. Rev.* A **39** 3053
[18] Chakrabarti A and Toral R 1989 *Phys. Rev.* B **40** 11 419
[19] Guo H, Grossmann B and Grant M 1990 *Phys. Rev. Lett.* **64** 1262
[20] Amar J and Family F 1990 *Phys. Rev.* A **41** 3399
[21] Hyman J M, Nicolaenko B and Zaleski S 1986 *Physica* **23D** 265
[22] Zaleski S 1989 *Physica* **34D** 427
[23] Kolb M 1987 *J. Phys. A: Math. Gen.* **20** L285
[24] Guo H, Grossmann B and Grant M 1990 *Phys. Rev.* A **41** 7082
[25] Tang L H, Nattermann T and Forrest B M 1990 *Phys. Rev. Lett.* **65** 2422