March 1994 Dipartimento di Fisica dell'Università di Pisa IFUP-TH 16/94

Numerical simulation of the Kardar-Parisi-Zhang equation

Matteo Beccaria[1,2] Giuseppe Curci[2,1]

(1) Dipartimento di Fisica, Universitá di Pisa
Piazza Torricelli 2, I-56100 Pisa, Italy

(2) I.N.F.N., sez. di Pisa
Via Livornese 582/a, I-56010 S. Piero a Grado (Pisa) Italy

Abstract

We simulate the Kardar-Parisi-Zhang equation in 2+1 dimensions. It is a non linear stochastic differential equation which describes driven growing interfaces. The Hopf-Cole transformation is used in order to obtain a stable numerical scheme. The two relevant critical exponents are precisely measured.

PACS numbers: 64.60.Ht, 05.40.+j, 05.70.Ln, 68.35.Fx

1. Introduction

Growing surfaces exhibit a non equilibrium critical dynamics with scaling properties similar to those of equilibrium critical phenomena. Many models have been proposed to describe the universal features of the growth process. The first numerical investigations [1] showed that the critical behaviour of the surface is described by two exponents z and χ. The interface roughness W (to be defined later) grows with time t as

$$W \sim L^{\chi} f\left(t\ L^{-z}\right) \tag{1}$$

where L is the system size. Among the possible systems possessing such a scaling law, we mention for instance lattice ballistic deposition models, lattice stacking models or Eden clusters. In [2], Kardar, Parisi and Zhang (KPZ) proposed a non linear stochastic differential equation to describe growing interfaces. Non linearity was related to lateral growth of the interface. The dynamic Renormalization Group analysis [2, 3, 4] determined the flow of the non-linearity parameter λ related to the deposition speed. The exponents χ and z depend on the particular fixed-point λ^* which is reached asymptotically. Dimensionality of space is a priori relevant. If $\lambda^* \neq 0$, the hyperscaling relation $\chi + z = 2$ holds perturbatively. In $d = 1$ (growth on a line), the lowest order values for the exponents

$$z = \frac{3}{2} \qquad \chi = \frac{1}{2} \qquad \beta = \frac{\chi}{z} = \frac{1}{3} \tag{2}$$

can be shown to be exact [2] and are supported by several numerical simulations on the various models listed above. In $d = 2$, the perturbative Renormalization Group analysis breaks down, the flow is toward a strong coupling fixed-point and numerical simulation becomes very interesting. Kardar, Parisi and Zhang conjectured [2] the χ, z exponents to be superuniversal, namely independent on d, but they did not give analytical arguments. Successive works on the subject can be roughly divided into three groups. The first one deals with Eden cluster growth [5] and off lattice aggregation models with possible readjustement mechanisms [6]. The second group studies directed polymers [7] and RSOS (Restricted Solid on Solid) models [8] which are related to the KPZ equation. Finally, the third group simulates directly the KPZ equation by discretizing space and time and averaging over the realizations of the noise [9, 10, 11, 12].

Apart from the direct simulations of the KPZ equation, the information on the exponents extracted from the other models is somehow indirect. Indeed, directed polymers have been studied only in the zero temperature limit whereas the other models have not been shown rigorously to be in the same universality class of the KPZ equation. On the other hand, the direct simulation of the stochastic equation is hampered by great crossover effects which are relevant on the time scale actually explored in the simulations. Numerical instabilities are also potentially harmful.

In Tab.(1), I have collected estimates for χ and β coming from large scale simulations of Eden clusters [5], ballistic deposition models [6], directed polymers [7], RSOS models [8] and direct simulation of the KPZ equation [12](the χ exponent is taken from [10]). I have also shown the $d = 1$ exponents and the conjecture of Kim and Kosterlitz [13]

$$\chi = \frac{2}{d+3} \qquad \beta = \chi/z = \frac{1}{d+2} \tag{3}$$

based empirically on RSOS simulations in various dimensionalities. The situation in $d = 2$ is therefore the following: (i) the hyperscaling relation has strong numerical support and (ii) the exponents seem to rule out the superuniversality hypotesis and agree reasonably well with the prediction of [13].

Up to date, the most precise data on β, χ coming from direct simulations of the KPZ equation are those of [12] who however did not check $\chi + z = 2$. The authors of /citeMoser complain about numerical instabilities arising at large non-linearity: this unpleasant situation forced them to utilize very small integration steps not required in order to reduce the systematic error due to finite integration step. In this work we propose the simulation of the KPZ equation after the Hopf-Cole transformation which improves numerical

	χ	β
Eden	0.39(3)	0.22(3)
Ballistic	$\sim 1/3$	$\sim 1/4$
Polymers	0.53(7)	0.33(2)
KPZ	~ 0.38	0.240(5)
RSOS	0.385(5)	0.240(1)
KK	2/5	1/4
$d = 1$	1/2	1/3

Table 1: Summary of the $d = 2$ results.

stability due to the elimination of the non-linear term. We measure β and χ with high statistics and confirm the results of [12].

2. The Renormalization Group analysis of the Kardar-Parisi-Zhang equation

The Kardar-Parisi-Zhang equation [2] in d dimensions for the interface height $h(x,\ t)$ is

$$\frac{\partial h}{\partial t} = \nu\ \nabla^2 h + \frac{\lambda}{2} (\nabla h)^2 + \eta(x,\ t) \qquad x \in \mathrm{R}^d \tag{4}$$

The noise η is gaussian and the associated diffusion D

$$\langle \eta(x_1,\ t_1)\ \eta(x_2,\ t_2) \rangle = 2\ D\ \delta^{(d)}(x_1 - x_2)\ \delta(t_1 - t_2) \tag{5}$$

is a constant. The relaxation term in Eq.(4) provides the surface tension responsible for molecular readjustement. The non linear term is related to lateral growing of the interface. The KPZ equation is actually a truncated gradient expansion: therefore, full invariance under tilts is lost. However, the infinitesimal symmetry

$$h \to h + \varepsilon \cdot x \qquad x \to x + \lambda\ t\ \varepsilon \qquad \varepsilon \text{ infinitesimal} \tag{6}$$

is unbroken. Indeed, if $h(x,t)$ is a solution, then also

$$h(x + \lambda\ t\ \varepsilon,\ t) + \varepsilon \cdot x \tag{7}$$

is a solution up to $O(\varepsilon)$. Let us introduce large scale variables

$$\tilde{x} = x/l \qquad \tilde{t} = t/l^z \tag{8}$$

where l is a length scale. Given a solution $h(x,\ t)$ corresponding to parameters $(\nu,\ \lambda,\ D)$, the function

$$\tilde{h}(\tilde{x},\ \tilde{t}) = l^{-\chi}\ h(x,\ t) = l^{-\chi}\ h(l\ \tilde{x},\ l^z\ \tilde{t}) \tag{9}$$

is a solution corresponding to new parameters $(\tilde{\nu},\ \tilde{\lambda},\ \tilde{D})$ where

$$\tilde{\nu} = l^{z-2}\ \nu \qquad \tilde{\lambda} = l^{\chi+z-2}\ \lambda \qquad \tilde{D} = l^{z-d-2\chi}\ D \tag{10}$$

Therefore, for $d > 2$, we have the critical exponents

$$z = 2 \qquad \chi = \frac{2-d}{2} \tag{11}$$

and an asymptotically ideal surface with $\lambda = 0$. To explore $d \leq 2$ we need a one loop analysis. The evolution equations change into

$$\begin{aligned}
\nu'(l) &= \left(z - 2 + K_d \bar{\lambda}^2 \frac{2-d}{4d}\right)\ \nu && (12)\\
\lambda'(l) &= (\chi + z - 2)\ \lambda && (13)\\
D'(l) &= \left(z - d - 2\chi + K_d \frac{1}{4} \bar{\lambda}^2\right)\ D && (14)
\end{aligned}$$

where $\bar{\lambda} = \lambda^2 D/\nu^3$ and $K_d = S_d/(4\pi)^d$. The second equation does not get perturbative corrections. This is a non trivial consequence of the infinitesimal tilt invariance. It is a well known result of fluctuating hydrodynamics [3]. It follows that the hyperscaling relation $\chi + z = 2$ must hold at a non trivial critical point. The running $\bar{\lambda}$ satisfies[1]

$$\bar{\lambda}' = \frac{2-d}{2}\,\bar{\lambda} + K_d\frac{2d-3}{4d}\,\bar{\lambda}^3 \tag{15}$$

The usual ε-expansion at the non-trivial $O(\varepsilon)$ fixed point gives at $d=1$ the exponents

$$d = 1 \qquad z = \frac{3}{2} \qquad \chi = \frac{1}{2} \tag{16}$$

Furthermore, in $d = 1$ a fluctuation-dissipation theorem [14] can be invoked stating that at all orders of perturbation theory the renormalizations of the evolution equations of ν and D are equal. Therefore, the above exponents are exact.

However, at the critical dimension $d = 2$, the flow is beyond pertubation theory with λ growing as l increases and going eventually to an unknown strong coupling fixed point.

3. W and crossover

The measure of β, χ is done by looking at the interface roughness defined as

$$W = \langle h^2\rangle_c = \langle h^2\rangle - \langle h\rangle^2 \tag{17}$$

where the average is over the lattice and $W(t, L)$ is averaged over the noise. At the unstable trivial fixed point $\lambda = 0$, the growth is marginal and follows the law

$$W^2 \sim A\ \ln t \tag{18}$$

Starting from $\lambda \neq 0$, we expect to observe the asymptotic scaling

$$W \sim t^\beta \tag{19}$$

in infinite volume. Finite size effects allow the observation of Eq.(19) only as an intermediate regime and at $t \to \infty$ we have saturation with $W \to W_{\rm sat}(L)$.

[1]The evolution equation Eq.(12) does not change the naive results of Eq.(11) since $\lambda = 0$ is still stable. However a transition at large λ is possible in principle.

The determination of β is rather difficult. If λ is too large, a small integration step is needed to keep the systematic error small. If, on the other hand, λ is small, crossover is observed with the scaling Eq.(19) setting up slowly at small λ. Moreover, saturation effects must always be kept under control by comparing data obtained on larger and larger lattices.

4. Discretization and the Hopf-Cole transformation

We rescale time and h in order to reduce the number of independent parameters in the KPZ equation. Its canonical form is thus

$$\frac{\partial h}{\partial t} = \nabla^2 h + \sqrt{\lambda}\,(\nabla h)^2 + \eta(x,\ t) \tag{20}$$

with[2]

$$\langle \eta(x_1,\ t_1)\ \eta(x_2,\ t_2)\rangle = \delta^{(d)}(x_1 - x_2)\ \delta(t_1 - t_2) \tag{21}$$

and where we have changed variable

$$\frac{2\lambda^2 D}{\nu^3} \to \lambda \tag{22}$$

The equation depends thus on only one parameter which determines the degree of non linearity. The quadratic term $(\nabla h)^2$ is responsible for numerical instabilities since the typical surface becomes more and more rough. We propose to utilize the Hopf-Cole transformation (see [15] for a different application)

$$h = \frac{1}{\sqrt{\lambda}}\ \ln w \qquad w = \exp\left(\sqrt{\lambda} h\right) \tag{23}$$

At a formal level, this gives a diffusion equation with multiplicative noise

$$\dot{w} = \nabla^2 w + \sqrt{\lambda}\ w\ \eta(x,\ t) \tag{24}$$

[2] η is a gaussian noise in the following discussion, but in a lowest order integration scheme, like the Euler one, it can always be replaced by a uniform random number with the same first two momenta. The same trick is used in [10] where the invariance of the results is explicitely checked.

In principle, there are ambiguities in the discretization of Eq.(24) because the noise is not differentiable. To be general, let us consider the following stochastic equation for $h(x,\ t) : R^d \times R \to R$

$$\dot{h} = f(h) + \xi \qquad \langle \xi(t_1)\xi(t_2)\rangle = \delta(t_1 - t_2) \tag{25}$$

Its precise interpretation is the discrete process

$$\begin{aligned} h_{n+1} &= h_n + \varepsilon f(h_n) + \sqrt{\varepsilon}\ \xi_n && (26) \\ \xi_n &: \text{normal random variables} && (27) \end{aligned}$$

and averages over the stochastic realizations must be extrapolated to the $\varepsilon \to 0$ limit. The result of a general transformation of h is well understood in terms of the corresponding Fokker-Planck equations. If $P_h(h,t)$ is the density of processes relative to Eq.(25), we have

$$\frac{\partial P_h}{\partial t} = \frac{1}{2}\frac{\partial^2 P_h}{\partial h^2} - \frac{\partial}{\partial h}\left(f(h)P_h\right) \tag{28}$$

We now consider the change of variables $h = \ln w$ (the following reasoning is however completely general, provided that the change of variables is well defined). P_h is a density and transforms accordingly as

$$P_h = \left|\frac{\partial w}{\partial h}\right| P_w = wP_w \tag{29}$$

Substituting into Eq.(28) we obtain

$$\frac{\partial P_w}{\partial t} = \frac{1}{2}\frac{\partial^2}{\partial h^2}(w^2 P_w) - \frac{\partial}{\partial h}\left[w(f(\ln w) + 1/2)P_w\right] \tag{30}$$

A simple discrete process which in the $\varepsilon \to 0$ limit gives rise to Eq.(30) is

$$w_{n+1} = w_n + \varepsilon\ w_n\ \left[f(\ln w_n) + \frac{1}{2}\right] + \sqrt{\varepsilon}\ w_n\ \xi_n \tag{31}$$

The same result is obtained by applying directly the Hopf-Cole transformation to the Euler discretization of the original equation. Here, the additional term in the force is not $1/2$, but $1/2\xi_n^2$; of course, there is no difference.

We remark that we have eliminated all the potential ambiguities related to the choice of Ito or Stratanovitch calculus since we have constructed explicitely our stochastic processes, by their unambiguous discrete realizations.

5. The simulation

The numerical simulation has been done on the APE supercomputer [16]. The model operating at Pisa is the so called "tube" machine, a 128 processor parallel computer with a peak performance of 6 GigaFlops. We have simulated the $d = 2$ growth process on a square lattice with sizes up to $L = 512$. Every integration of the KPZ equation was averaged over 128 realizations of the noise. The value of the integration step was chosen in order to have irrelevant differences with smaller values. In Fig.1, we show (from top to bottom) the behaviour of W at $\lambda = 25, 10, 7.5, 5, 2$; we have used $\varepsilon = 5 \cdot 10^{-4}, 10^{-3}, 2.5 \cdot 10^{-3}$ for the first three and $\varepsilon = 5 \cdot 10^{-3}$ for the others. At $\lambda = 25$ we have taken data on the $L = 512$ lattice, the other values are at $L = 256$. The crossover effect inducing effective exponents is evident in the figure. In order to avoid finite size effects, we determined β over a range where changing L from 256 to 512 was irrelevant. We obtained $\beta = 0.240(1)$. The exponent χ has been obtained by studying the saturation width as a function of L by mean of long runs. The points in Fig.2 give $\chi = 0.404(1)$. Therefore, the hyperscaling relation is well satisfied. Our results are compatible with [12] and with the empirical conjecture of [13]. Of course, we cannot be sure to have eliminated totally the crossover effects. The common lore is that, due to saturation effects, numerical estimates for β must be considered lower bounds. It is clear that, even if the agreement with RSOS models is encouraging, an analytical upper bound would be desirable.

7. Conclusions

The main goal of this paper has been an high statistics simulation of the KPZ equation put in an alternative form after the Hopf-Cole transformation. This change of variables in the stochastic equation does not present any problem from the point of view of the simulations and is numerically stable. Our measures of β and χ satisfy the hyperscaling relation and are compatible with the conjecture of [13].

Acknowledgements

We thank Prof. Raffaele Tripiccione for a continuous help in developing the codes for the APE machine.

References

[1] F. Family and T. Vicsek, J. Phys. A (1985) L75.

[2] M. Kardar et al., Phys. Rev. Lett. 56 (1986) 889.

[3] E. Medina et al., Phys. Rev. A39 (1989) 3053.

[4] D. Forster, D. R. Nelson and M. J. Stephen, Phys. Rev. A 16 (1977) 732.

[5] P. Devillard and H. E. Stanley, Physica A160 (1989) 298.

[6] R. Jullien and P. Meakin, Europhys. Lett. 4 (1987) 1385.
P. Meakin et al., Phys. Rev. A34 (1986) 5091.

[7] M. Kardar and Y-C. Zhang, Phys. Rev. Lett. 58 (1987) 2087.

[8] B. M. Forrest and L-H. Tang, Phys. Rev. Lett. 64 (1990) 1405.

[9] A. Chackrabarti and R. Toral, Phys. Rev. B16 (1989) 11419.

[10] J. G. Amar and F. Family, Phys. Rev. A41 (1990) 3399.

[11] B. Grossmann et al., Phys. Rev. Lett. 64 (1990) 1262.
B. Grossmann et al., Phys. Rev. A41 (1990) 7082.
B. Grossmann et al., Phys. Rev. A43 (1991) 1727.

[12] K. Moser et al., Physica A178 (1991) 215.

[13] J. M. Kim and J. M. Kosterlitz, Phys. Rev. Lett. 62 (1989) 2289.

[14] U. Deker and F. Haake, Phys. Rev. A11 (1975) 2043.

[15] S. E. Esipov and T. J. Newman, Phys. Rev. E48 (1993) 1046.

[16] A. Bartoloni et al., Intl. Journal of Mod. Phys. C4 (1993) 969.