IIT, Bombay

EP 413 Mini-project
Autumn 2015

Study of scaling properties of surface growth

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Introduction

The aim of this project was to study the scaling properties of one dimensional Edward-Wilkinson and Kardar-Parisi-Zhang surfaces using simulations. A number of interesting phenomena can be described in terms of the motion of an interface between two phases of matter. Crystal growth, propagation of flame fronts, fluid displacement in porous media, and growth of bacterial colonies are a few examples which are important from both the theoretical and practical point of view. Despite the multitude of different microscopic mechanisms underlying these phenomena, they all exhibit remarkably similar growth dynamics.

There was a surge of activity in the field of surface dynamics in 1980s. Edward and Wilkinson proposed a model described by a linear Langevin equation. A seminal paper by Family and Viscek in 1985 on scaling of surfaces set the foundation for much of the future work. The theory of self-affine curves was being simultaneously developed by Mandelbrot, Voss and others. In a 1986 paper Kardar, Parisi, and Zhang (KPZ) proposed a nonlinear continuum equation for describing the dynamics of growing surfaces. This model correctly predicted the critical exponents of ballistic deposits. Although this is a non-equilibrium process, surface growth shows striking similarities with the critical behavior of phase transitions of systems in equilibrium.

Firstly a brief summary of the general principles of dynamic scaling and self-affinity is given. Theoretical treatment of the EW model is followed by the simulation results of the random deposition With surface relaxation model.. Rigorous theoretical analysis of the KPZ equation was not done due to shortage of time. Finally simulation results of the ballistic deposition model are reported.

Dynamic Scaling

We will be concerned with the study of *dynamics* of surface growth and *morphology* of resulting surfaces. A surface in $d+1$ dimensions is defined as the highest part of an aggregate formed by deposition of vertically falling particles. Substrate is assumed to be a dimensional horizontal lattice. All the surfaces in this report will be 1+1 dimensional. Height of a surface at a lattice site is the height of the corresponding column. Mean height and surface width are defined as,

$$\bar{h(t)} = \sum_{i=1}^{L} \frac{h(i,t)}{L}$$

$$w(L,t) = \sqrt{\frac{1}{L}(h(i,t) - \bar{h})^2}$$

where, $h(i,t)$ is the height of the 'i'th column and L is the length of the substrate. Width is a quantitative measure of the roughness of the surface.

For a general surface, the width evolves with time as shown in,. Width initially grows as a power law with time but eventually saturates after a crossover time $t_\times$. It follows the following laws,

$$w(L,t) \sim t^\beta \qquad t << t_\times$$

$$w_{sat}(L) \sim L^\alpha \qquad t << t_\times$$

$$t_\times \sim L^z$$

β is called the growth exponent, α the roughness exponent and z the dynamic exponent. These are not independent of each other as can be seen from,

$$w(t_\times) \sim t_\times^\beta \qquad w(t_\times) \sim L^z$$

Thus we get the scaling law,

$$z = \alpha/\beta$$

These laws suggest the following relation called the Family-Viscek scaling relation,

$$w(L,t) \sim L^\alpha f(t/L^z)$$

f is called the scaling function. It shows the following asymptotic behavior,

$$f(u) \sim u^\beta \qquad t << t_\times$$

$$f(u) = constatnt \qquad t >> t_\times$$

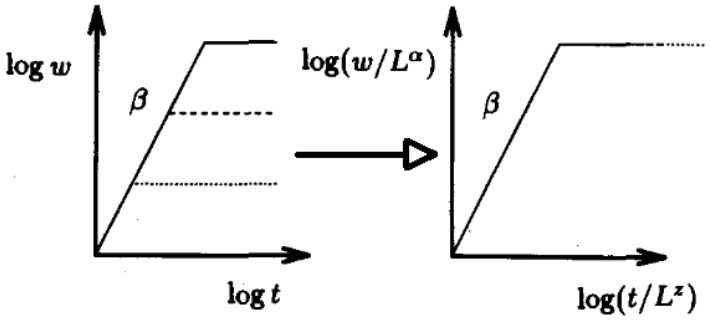

Figure 1: Collapse of surface width dynamics[1]

If w/w_{sat} is plotted against $t/t_\times$, the curves for different L values collapse onto the scaling function. The saturation of surface width is a consequence of height correlations spreading across the surface over time. From the scaling relations following can be deduced about the correlation length parallel to the surface,

$$\xi_{||} \sim t^{1/z} \qquad t << t_\times$$
$$\xi_{||} = L \qquad t >> t_\times$$

The height difference correlation function has the scaling form,

$$c(r,0) \sim r^{2\alpha} \qquad r << L$$

$$c(0,t) \sim t^{2\beta} \qquad t << t_\times$$

These three scaling exponents characterize the growth models and define the universality classes.

Self-affinity

The expressions describing the scaling properties of the surface width can now be used to treat the dynamic scaling of the surface itself. Let,

$$\bar{h}(r) = h(r)\bar{h},$$

which is the deviation of the surface from its average. The scaling laws suggest the following form for $\bar{h}(x)$,

$$\bar{h}(r) = t^\beta f(r/t^{1/z})$$

where,

$$f(x) \sim L^{-\alpha} f(Lx) \qquad y << 1$$
$$|f(x)| < 1 \qquad y >> 1$$

A function with these properties is called a self-affine function, with self-affine exponent α. This Relation formulates in general terms the fact that a self-affine function must be rescaled in a different way horizontally and vertically: if we 'blow up' the function with a factor b horizontally, it must be 'blown up' with a factor b" vertically in order that the resulting object overlaps the object obtained in the previous generation. A saturated surface satisfies this relation in a statistical sense and is thus termed a random self-affine fractal.

The dynamic scaling relation and the self-affine property of surfaces portray a striking similarity between surface growth dynamics and the critical state of equilibrium phase transitions.

Random deposition

The simplest growth model is when particles are randomly generated at a position and deposited at the top of the column underneath it. This is called the random deposition model (RD). The columns of a generated RD surface have no correlation with each other and thus each column grows independently. Because of this, we cannot expect the surface to reach any saturated state. The probability that a column has height h after the deposition of N particles is,

$$P(h, N) = \binom{N}{h} p^h (1-p)^{(N-h)}$$

Thus the width evolves as,

$$w^2(t) =< h^2 > - < h >^2 = \frac{N}{L}(1 - \frac{1}{L})$$

Therefore,

$$\beta = 2$$

α and β are not defined for this model. A stochastic continuum growth equation can be associated with RD,

$$\frac{\partial h}{\partial t} = F + \eta(x, t)$$

where F is the constant flux of particles and η is the uncorrelated noise satisfying,

$$< \eta(x,t) >= 0, \qquad < \eta(x,t)\eta(x',t') >= 2D\delta^d(x-x')\delta(t-t')$$

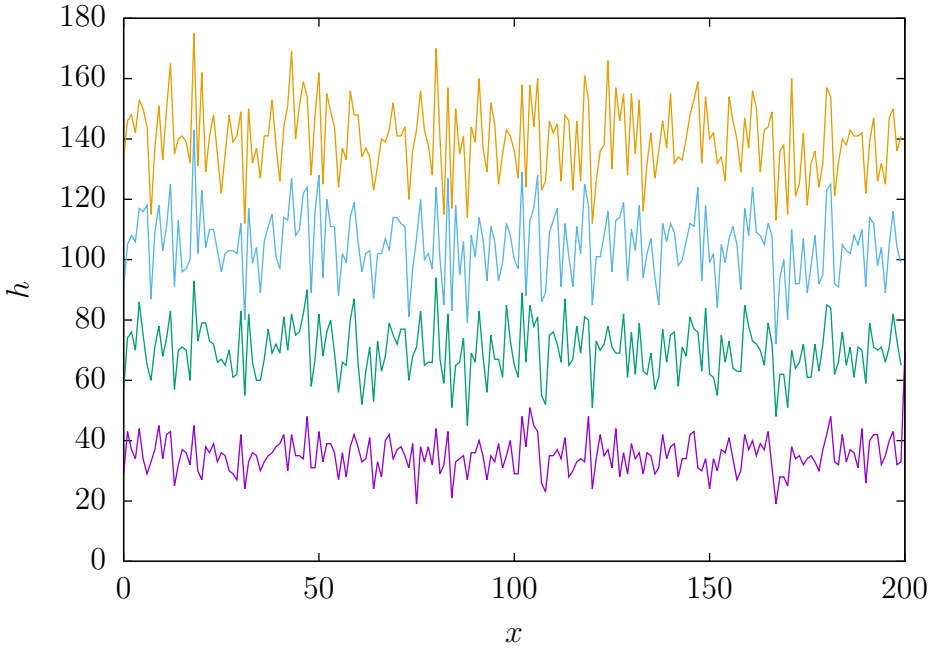

Figure 2: Surface height profile plotted after every 6000 depositions

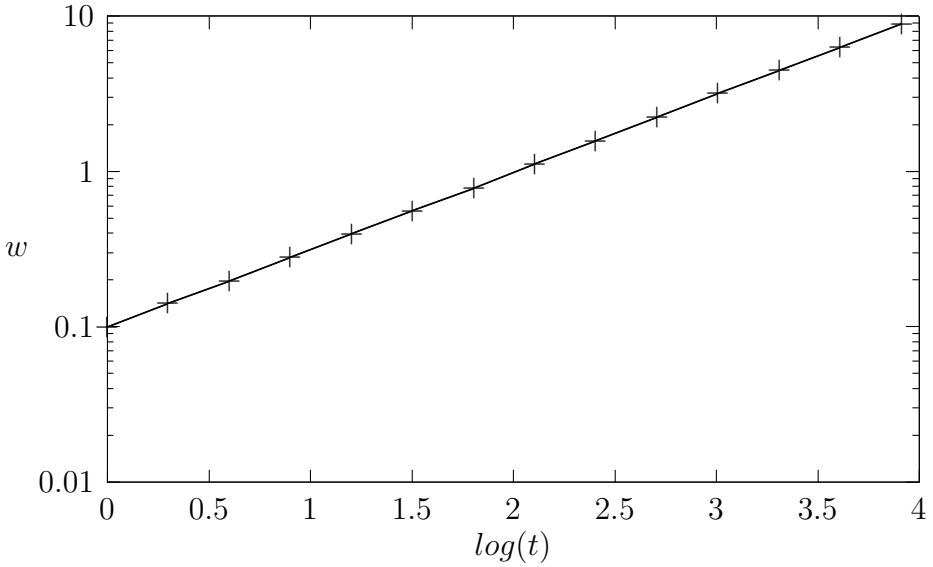

Figure 3: Surface width vs log(time) averaged over 100 simulations for $L = 200$. Log scale used on y axis

Integrating, we get,

$$h(x,t) = Ft + \int_o^t dt' \eta(x,t')$$

$$< h(x,t) >= 0 \qquad < h^2(x,t) >= F^2t^2 + 2Dt$$

Therefore,

$$w^2(t) = 2Dt \implies \beta = 2$$

$\beta = 0.498 \pm 0.003$ is found from simulations.

Edward-Wilkinson equation

In this section, the linear EW equation is discussed. First the corresponding discrete model called random deposition with surface relaxation is presented.

In order to account for the finite surface diffusion which exists in most of the realistic situations, in RDSR a deposited particle is allowed to diffuse around on the surface within a prescribed region about the column in which it was dropped until it finds the column with the smallest height. At this point the particle sticks to the top of that column and becomes part of the aggregate. This gives rise to correlations among different columns and leads to saturation of the width. Since, the results are found to be independent of extent of the allowed region of diffusion, only nearest-neighbor diffusion was allowed in the simulations. Periodic conditions are applied at the two ends.

Table 1: β for different L values

L	β
32	0.23
64	0.22
128	0.24
256	0.25

Values of the exponents found by simulations are,

$$\alpha = 0.48 \pm 0.01 \qquad \beta = 0.23 \pm 0.02 \qquad z = 2.07 \pm 0.10$$

The general form of growth equation is given by,

$$\frac{\partial h(\mathbf{x},t)}{\partial t} = G(h,\mathbf{x},t) + \eta(\mathbf{x},t)$$

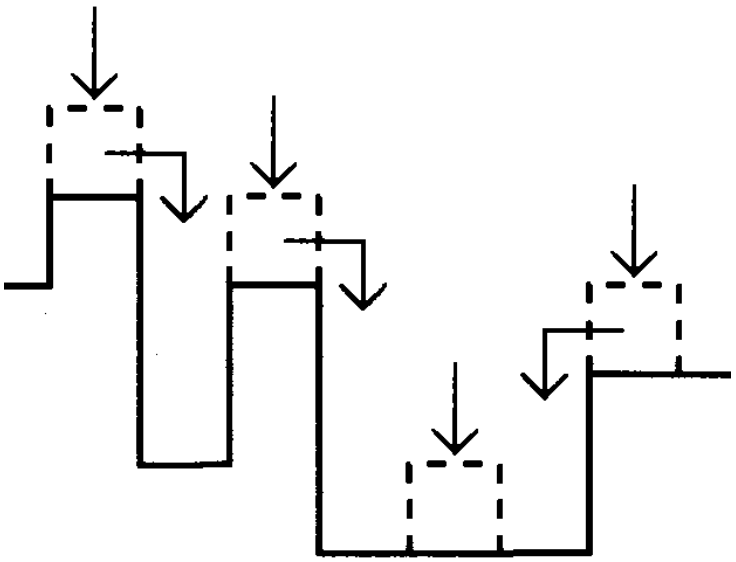

Figure 4: RDSR[1]

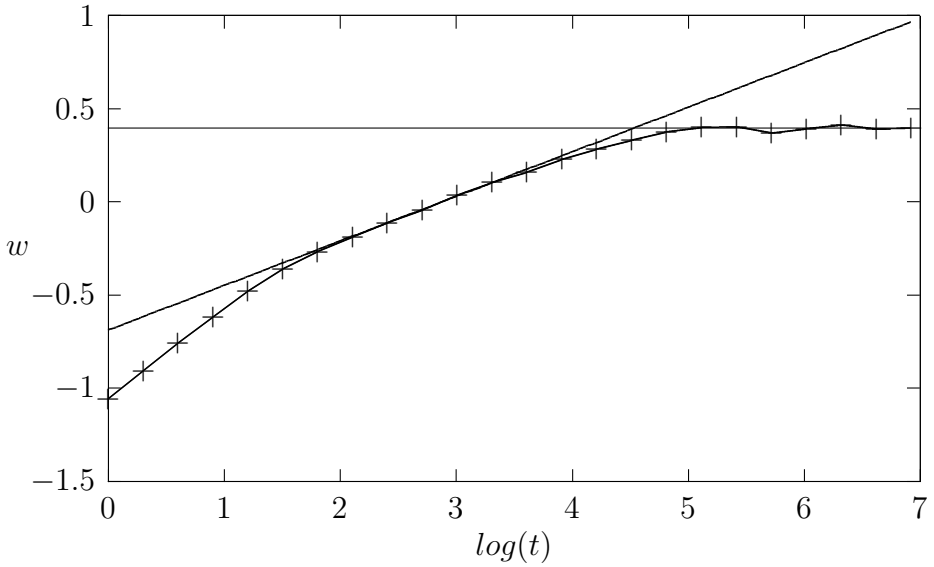

Figure 5: log(width) vs log(time) for $L = 128$ averaged over 100 simulations. As indicated in [3] there are three parts to this curve. Slope of linear fit $0.238865(\pm 0.0005)$ is close to the theoretical value of $\beta = 0.25$

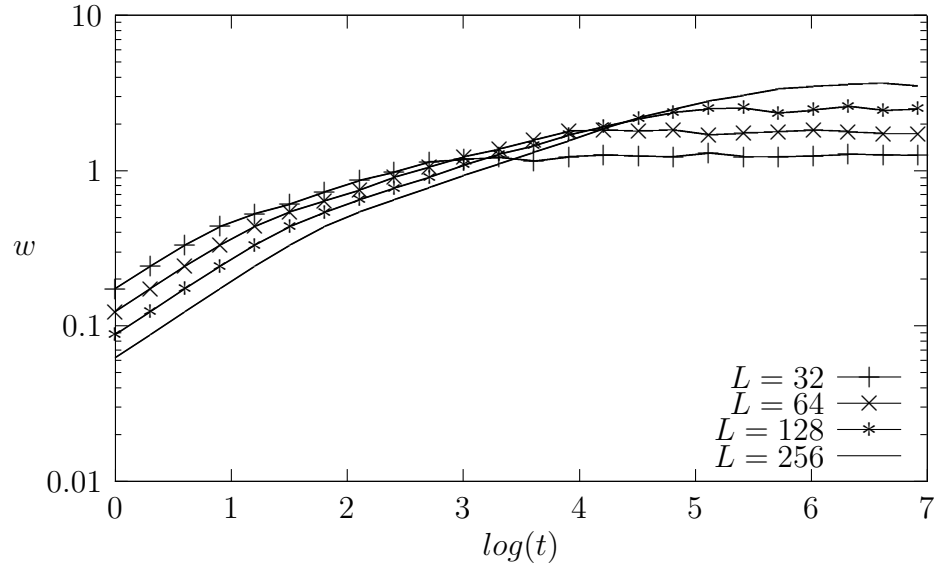

Figure 6: Width vs log(time) averaged over 100 simulations. Log scale used on y axis

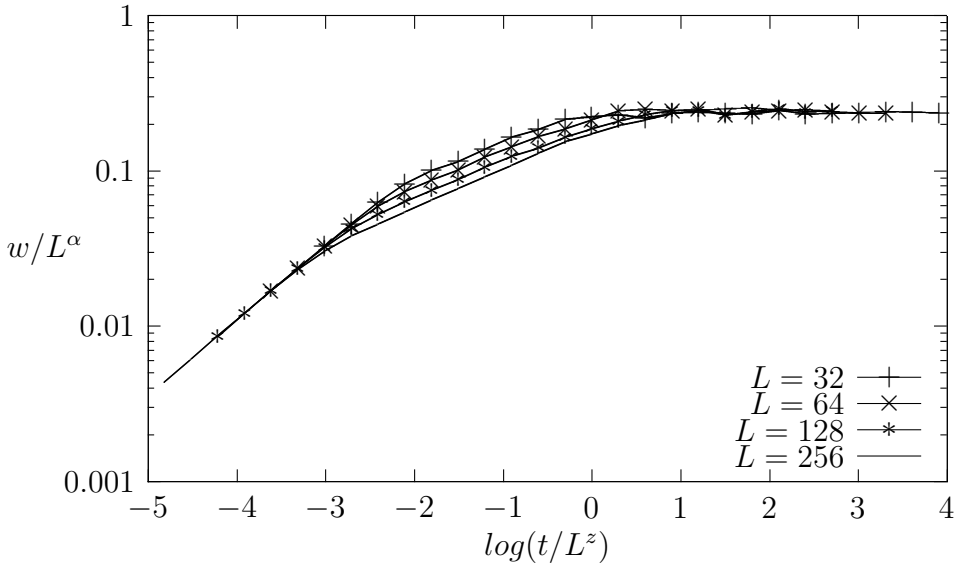

Figure 7: Scaled width vs log(time). Log scale used on y axis

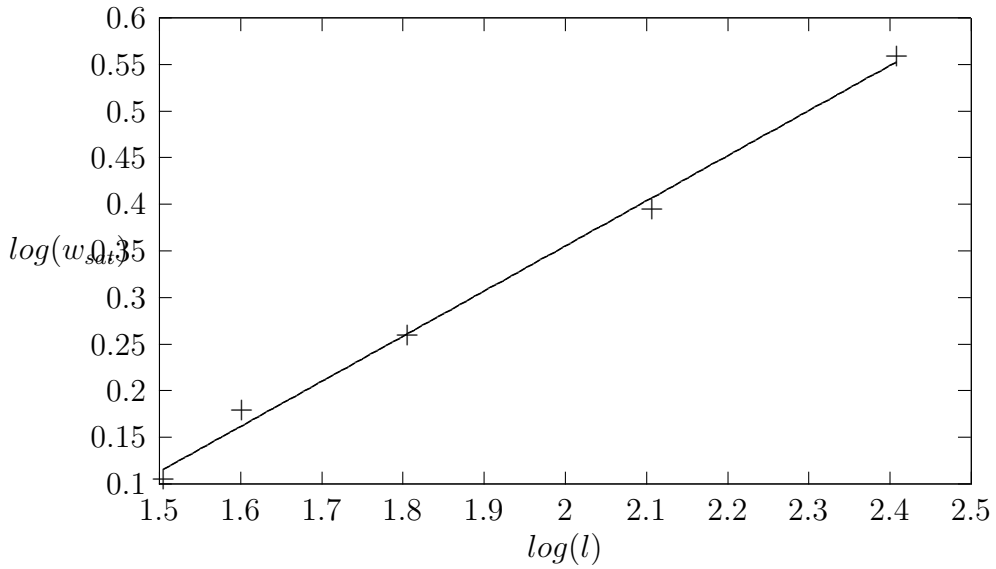

Figure 8: log(width) vs log(time). Slope of the linear fit is 0.48($\pm$0.01)

where η has the same properties as before. The form of the function $G(h, x, t)$ can be deduced from symmetry arguments. A surface in equilibrium should be invariant under the transformations,

$$t \to t + \delta t$$

$$h \to h + \delta h$$

$$\mathbf{x} \to \mathbf{x} + \delta \mathbf{x}$$

This means that the surface is independent of the origin of the coordinate system as well as the origin of time, since we should be able to study a surface from any point and any time and it should still behave consistently. For a surface not accounting for empty spaces inside the interface, it should also be symmetric about the origin of the coordinate system and the mean height which suggest invariance under the transformations,

$$h \to -h$$

$$\mathbf{x} \to -\mathbf{x}$$

Thus the allowed terms are,

$$\frac{\partial h(\mathbf{x}, t)}{\partial t} = \nabla^2 h + \nabla^4 h + ... + (\nabla^2 h)(\nabla h)^2 + ... + (\nabla^{2k} h)(\nabla h)^{2j} + \eta(\mathbf{x}, t)$$

In the hydrodynamic limit, higher order derivatives should be less important compared to the lowest order derivatives, which can be confirmed using scaling arguments. Renormalization group theory can be used to prove that excluding higher order terms does not alter the values of critical exponents. Thus the simplest equation is given by,

$$\frac{\partial h(\mathbf{x},t)}{\partial t} = \nu \nabla^2 h + \eta(\mathbf{x},t)$$

This linear Langevin equation is called the Edward-Wilkinson equation. ν is called the surface tension. The $\nabla^2 h$ term gives rise to diffusion along the surface. The average velocity of the interface is zero.

As EW equation is linear it can be solved exactly, but it is possible to extract the critical exponents from the equation using scaling arguments. Under the transformations,

$$x \to bx,\ h \to b^{\alpha} h,\ t \to b^{z} t$$

the equation should remain invariant[1]. Substituting these relations in the EW equation leads to,

$$\frac{\partial h(\mathbf{x},t)}{\partial t} = \nu b^{z-2} \nabla^2 h + b^{-d/2+z/2-\alpha} \eta(\mathbf{x},t)$$

Thus we get,

$$\alpha = \frac{2-d}{2} \qquad \beta = \frac{2-d}{4} \qquad z = 2$$

Exact solution obtained by fourier transforming gives,

$$< h(x,t)h(x',t') >= \frac{D}{2\nu} |x-x'|^{2-d} f(\nu \frac{|t-t'|}{|x-x'|^2})$$

which, gives the same values for the exponents. The values of exponents obtained from RDSR model and the EW equation match closely. Thus they belong to the same universality class known as the EW class.

Kardar-Parisi-Zhang Equation

First lets discuss the discrete ballistic deposition model (BD). A random lattice site is chosen, and a particle is deposited each time step. If the surface is higher at the points next to this chosen point, the particle will stick next

[1] It is not obvious that ν and D remain unchanged after scaling. This can be justified using dynamic renormalization group theory.

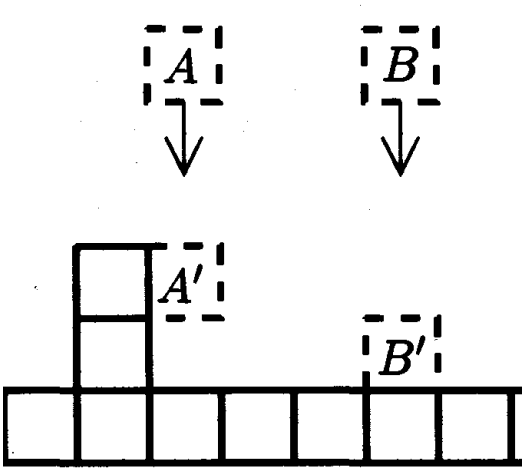

Figure 9: BD[1]

to the highest of these points, otherwise, it will stick to the surface at the same site.

$$h(i) = max[(h(i) + 1, h(i-1), h(i+1)]$$

Again periodic conditions are applied at endpoints. For smaller values of L, the domain of power law growth is very small, so it's hard to calculate β accurately. While this was true of the RDSR model too, here the L values are very large and take very long to saturate. Due to system hardware limitations it was not possible to do large scale simulations as done in [4]. So agreement with the theoretical values is not as good as for RDSR. Values

Table 2: β for different L values

L	β
256	0.28
512	0.31
1024	0.30

of the exponents found by simulations are,

$$\alpha = 0.42 \pm 0.02 \qquad \beta = 0.29 \pm 0.02 \qquad z = 1.45 \pm 0.10$$

EW does not account for growth that occurs at local normals of the surface. For a growth rate v along the surface normal, the increase in height is found to be,

$$\delta h = v\delta t(a + \nabla h^2)61/2$$

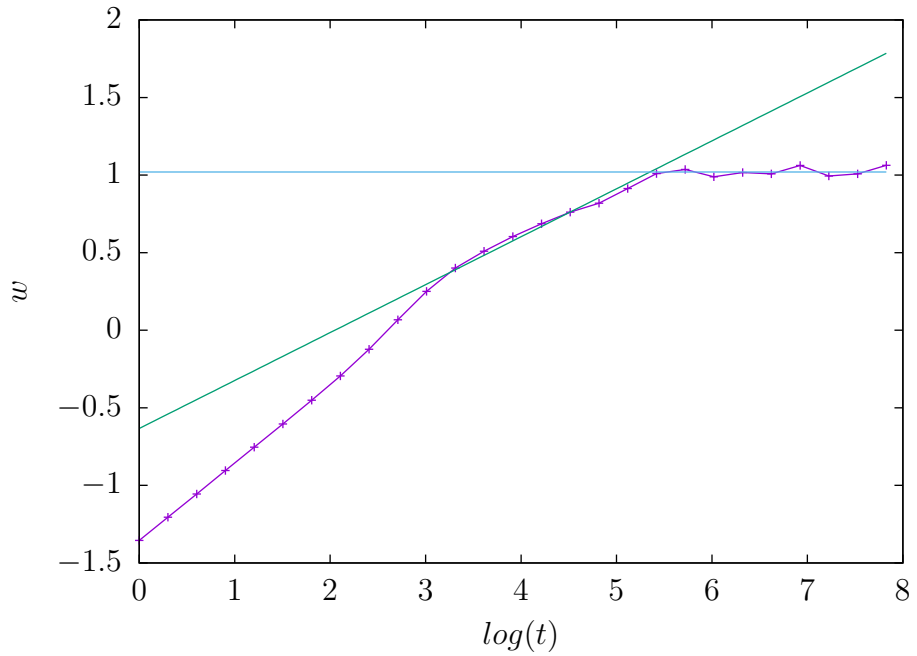

Figure 10: log(width) vs log(time) for $L = 512$ averaged over 50 simulations.

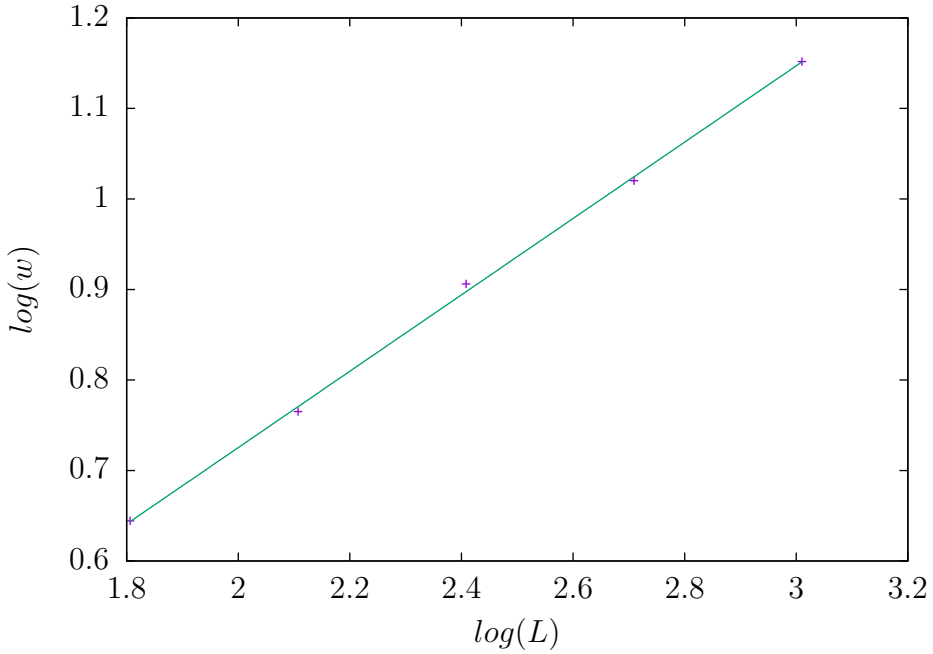

Figure 11: log(width) vs log(L) for calculation of α

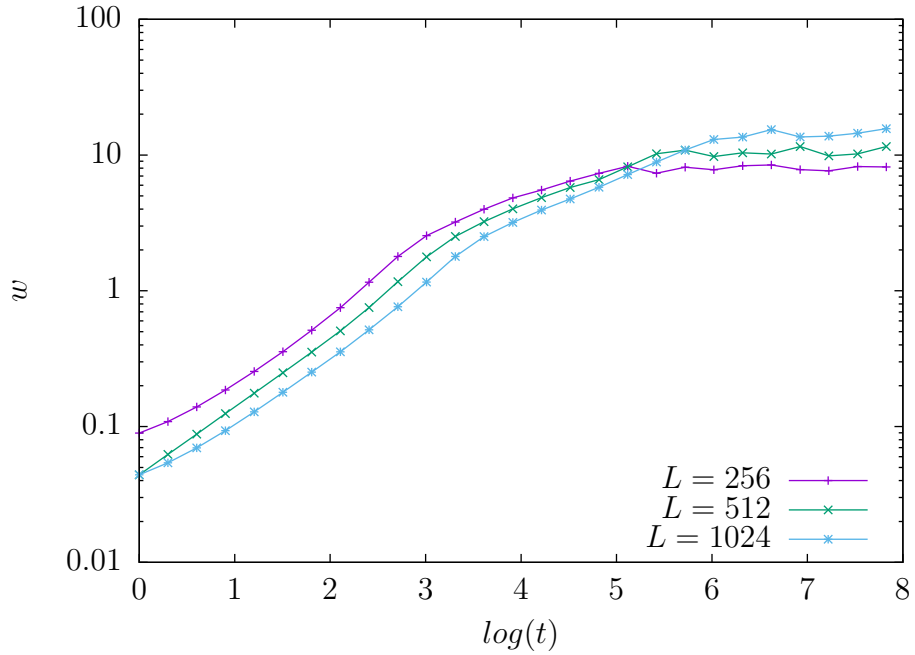

Figure 12: log(width) vs log(t) averaged over 50 simulations. Log scale used on y axis

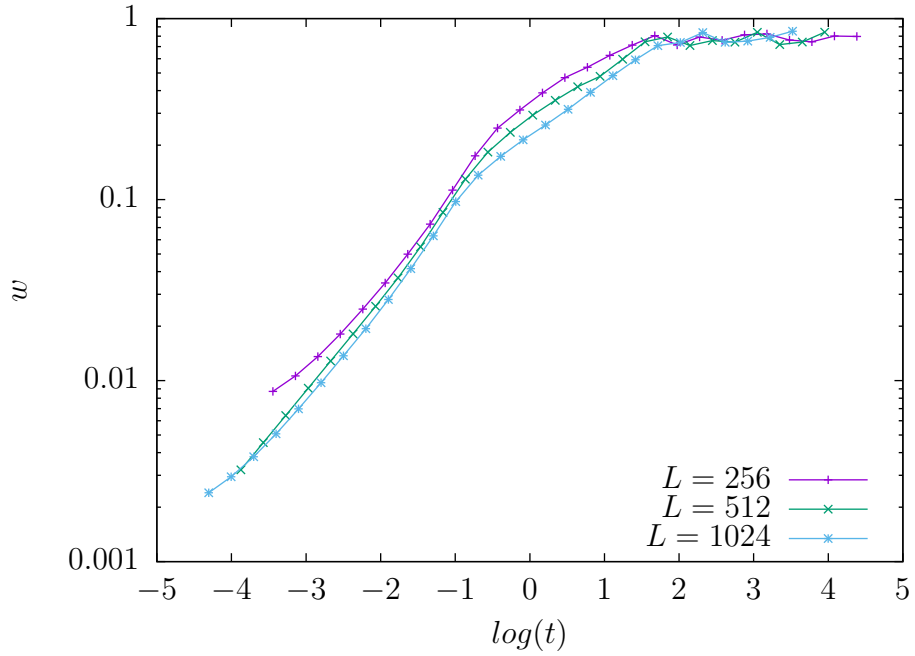

Figure 13: Scaled width vs log(t). Log scale used on y axis

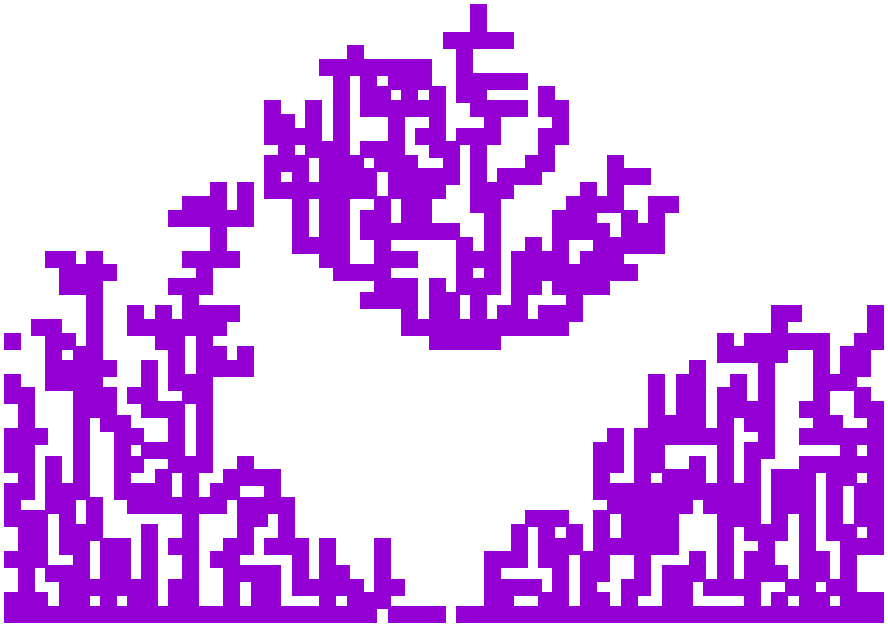

Figure 14: BD aggregate. Illustration of lateral propagation of correlations. Initially the surface has a peak in the middle.

for $|\nabla h| << 1$,

$$\frac{\partial h(\mathbf{x},t)}{\partial t} = v + v(\nabla h)^2 + \eta(\mathbf{x},t)$$

The $(\nabla h)^2$ term represents lateral growth observed on BD. The KPZ equation is,

$$\frac{\partial h(\mathbf{x},t)}{\partial t} = \nu\nabla^2 h + \frac{\lambda}{2}(\nabla h)^2 + \eta(\mathbf{x},t)$$

Due to the lateral growth property the $h \to -h$ symmetry is broken in KPZ equation. An interface governed by the KPZ equation has nonzero velocity even in the absence of an external driving force unlike the EW equation. The material added by the nonlinear term generates the excess velocity.

Using the same scaling arguments as before gives,

$$\frac{\partial h(\mathbf{x},t)}{\partial t} = \nu b^{z-2}\nabla^2 h + \frac{\lambda}{2} b^{\alpha+z-2}(\nabla h)^2 + b^{-d/2+z/2-\alpha}\eta(\mathbf{x},t)$$

This provides three scaling relations for the two exponents, thereby overdetermining them. Also in this case the constants change under rescaling. The correct values of the exponents can be found from renormalization theory as

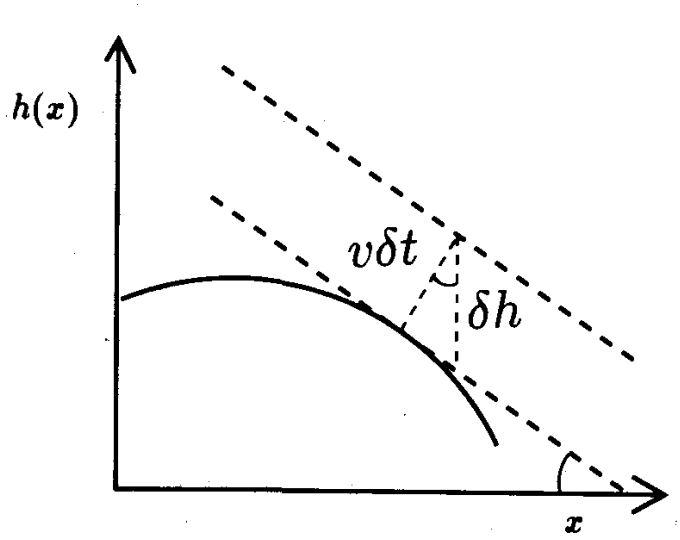

Figure 15: Growth normal to the surface[1]

(in 1+1 dimension);

$$\alpha = \frac{1}{2}, \qquad \beta = \frac{1}{3}, \qquad z = \frac{3}{2}$$

References

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