Dynamics of Fractal Functions

Doktori (PhD)értekezés

Müszaki informatikai alkalmazások
doktori program

Determinisztikus és sztochasztikus dinamikus
rendszermodellek alprogram

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Contents

Abstracts

Fraktálfüggvények dinamikája

A fraktálfüggvények dinamikájára vonatkozó vizsgálataink a fizika és a matematika határterületéhez tartoznak, gyakran a számítógépes szimulációt használva eszközül. A fraktálfelület–növekedés dinamikáját elsősorban a fizikai folyamat lényegét leíró egyenletek (sztochasztikus és determinisztikus parciális differenciálegyenletek - PDE) segítségével tanulmányoztuk.

A fizikai kísérletekhez kapcsolódó sztochasztikus növekedési modellek esetében célunk az volt, hogy olyan modellt találjunk, amely a kísérleti felülethez mennyiségileg is jól leírhatóan hasonló önaffin fraktálfelületet hoz létre. Új, multiplikativ befagyott zaj tag sztochasztikus parciális differenciálegyenletet írtunk fel és vizsgáltunk numerikus módszer segítségével. Modellünk a kísérleti eredményekkel nagyon jó egyezést mutat.

Célunk az instabil vagy szinguláris tagot tartalmazó determinisztikus PDE esetében már magának az egyenlet megoldásának numerikus és szimbolikus vizsgálata volt. A kapott komplex térido–viselkedést a fraktálfüggvények dinamikájával, az ott felhasznált módszerek segítségével írtuk le.

A sztochasztikus felületnövekedést szimuláló rácsmodellek megértését segítette elő az a programcsomagunk, amelyet 1992-ben a World Scientific kiadó publikált. Megjelenésekor ez a maga nemében első ilyen programcsomag volt, tartalmazta a modellek leírását és forrásnyelvu programjukat is. Azóta több száz példányát sikerrel használták elsősorban az oktatásban, esetenként kutatásra.

Dynamics of Fractal Functions

The dynamics of fractal functions is related to physics and mathematics as well, while in many cases we use computer simulation as a tool. The growth of fractal surfaces is mostly investigated by phenomenological equations (stochastic or deterministic partial differential equations — PDE) describing the physical process.

In the case of stochastic growth models related to physical experiments our aim was to find a model producing self affine fractal surfaces similar to the observed ones. By numerically solving our new, stochastic PDE with multiplicative quenched noise term we have obtained fractal surfaces which are in good agreement with the experimental interfaces.

We investigated a deterministic PDE with instable or singular terms numerically and simbolically as well. In this case we described the complex behaviour of the solutions in space and time also by the dynamics of fractal functions.

Our program package published in 1992 by World Scientific was the first one of its kind containing the description of the lattice models simulating fractal growth and their source code as well. Since that it was used mostly for educational purposes and small scale research.

Dynamik von fractal Funktionen

Die Dynamik von fractal Funktionen hängt mit Physik und Mathematik zusammen, während in vielen Fällen wir Computersimulation als Hilfsmittel verwenden. Das Wachstum der fractal Oberflächen meistens nachgeforscht durch die phänomenologischen Gleichungen (stochastische oder deterministische teilweise Differentialgleichungen - PDE) den Kern von physikalischen Prozess beschreiben.

Im Fallen der stochastischen Wachstummodelle, die auf Systemtestexperimenten war unser in Verbindung gestanden wurden, Ziel, einen vorbildlicher produzierenden Selbst zu finden, die fractal Oberflächen zu läutern, die beobachteten ähnlich sind. Indem wir numerisch unser neues, stochastisches PDE mit multiplikativer gelöschter Geräuschbezeichnung lösten, haben wir fractal Oberflächen erhalten, die im Einverständnis mit den experimentellen Schnittstellen sind.

Wir forschten ein deterministisches PDE mit den instable oder einzigartigen Bezeichnungen numerisch und simbolically ausserdem nach. In diesem Fall beschrieben wir das komplizierte Verhalten der Lösungen im Raum und in der Zeit auch durch die Dynamik von fractal Funktionen.

Unsere Programmeinheit veröffentlichte 1992 durch World Scientific war die erste seiner Art, welche die Beschreibung der Gittermodelle fractal Wachstum und ihren Quellencode ausserdem simulierend enthält. Seit dem, dass es wurde verwendet meistens für pädagogische Zwecke und Forschung

Chapter 1

Introduction

During the late 1980-ies "there has been an explosion of activity in the field of dynamics of fractal surfaces, which, — through the convergence of important results from computer simulations, analytical theories and experiments, — has led to significant advances in our understanding of nonequilibrium surface growth phenomena" [11].

A rich variety of natural and technological processes leads to the formation of complex interfaces. If the conditions of the growth processes are such that the development of the interface is only marginally stable and the fluctuations are relevant, the resulting structure is a rough surface and can be well-described in terms of nowhere differentiable, single-valued self-affine fractal functions.

A self-affine (fractal) function h has the property

$$h(x_1, ..., x_n) = \lambda_1^{-\alpha_1} ... \lambda_n^{-\alpha_n} h(\lambda_1 x_1, ..., \lambda_n x_n)$$

where α_i is called the roughness or Hurst exponent [2]. Typically there is only one characteristic roughness exponent α and the x_i are equivalent from the point of view of scaling and we can write a simpler form for any λ

$$h(x) = \lambda^{-\alpha} h(\lambda x), \quad x \in \mathbb{R}^n.$$

For a single variable x this property expresses the fact that the function is invariant under the following rescaling: shrinking along the x axis by a factor of $1/\lambda$, followed by rescaling of the values of the function (measured in the perpendicular direction) by a different factor $\lambda^{-\alpha}$.

The **dynamics of fractal surfaces** can be investigated by the help of simplified lattice models or by phenomenological equations (stochastic or deterministic partial differential equations) describing the physical process.

The surface growth is generally modeled by the Kardar, Parisi, Zhang (KPZ) equation [13]

$$\frac{\partial h}{\partial t} = \nu_0 \nabla^2 h + \lambda/2(\nabla h)^2 + \eta(x,t).$$

The KPZ equation shows the time dependence of the height $h(x,t)$ on the spatial derivatives of the surface. After some time the initially flat surface ($h(x,0) = 0$) becomes rough and can be described by the help of fractal geometry and fractal functions. Here ν_0 is a constant (related to the surface tension) and η is a noise term. In the original KPZ η is an uncorrelated Gaussian noise with zero-mean.

During the years the continuum equation approach has been developing through (a) numerous studies of the original equation and (b) investigations of closely related other equations containing further terms.

Our investigations are related to physics and mathematics as well, while in many cases we use computer simulation as a tool. We carried on research in **two main directions**. Both stochastic and deterministic growth models were described by PDEs. In case of the stochastic PDE we started from a flat surface, while for deterministic models the initial surface was different from zero.

We investigated some **stochastic growth models related to physical experiments** (of wetting fronts). Our goals were (i) to make assumptions which are as close to the experimental conditions as possible, (ii) to numerically investigate the resulting equation and (iii) to compare the obtained behaviour with that observed in the experiments. We proposed a modified KPZ type equation and we have obtained surfaces remarkably similar to those observed in the experiments [27],[28].

We were also interested in **deterministic models producing complex spatio-temporal behaviour**. In a recent approach to d dimensional complex spatio-temporal behaviour the various functions associated with these structures are considered as growing rough surfaces in a $d+1$ dimensional space [25]. This development connects the studies of growing fractal surfaces to the research how stochastic spatio-temporal behaviour emerges in more complex deterministic processes.

We studied the simplest family of deterministic PDEs producing growing fractal surfaces. These equations originally proposed by Zhang [17] have the forms

$$\frac{\partial h(x,t)}{\partial t} = \nabla^2 h(x,t) + \text{nonlinear term}$$

where several form of the singular term can be used, including

$$|\nabla h|^\alpha \qquad \text{with} \qquad \alpha < 1 \qquad \text{or} \qquad \ln(|\nabla h|).$$

Here we usually start from a random (or periodic) surface, (e.g., $h(x,0)$ is a random surface with heights uniformly distributed between 0.0 and 0.01). Physicists and mathematicians alike studied the Zhang equations, however, inspite of its simple form the complex behaviour of the solutions (even their existence, stability etc.) are not well understood mathematically. We could obtain analytic results — special solutions — for the equation with the logarithmic term [31].

In addition, we investigated the parameterized versions of the Zhang equations numerically. We showed that the discretized versions exhibit rich spatio-temporal behaviour representing a mixture of stochastic and deterministic regimes (see Figures 3.5,3.10). Varying the relative weight of the singular term we have been able to detect transitions in the global behaviour of the solutions [29].

The dissertation consists of the following parts. In Chapter 2 the theoretical background (both mathematical and physical) of the dynamics of fractal functions is presented. Here we review very briefly the basic mathematical ideas and notations concerning fractals used in our physical applications. We also present the main physical principles (as the dynamical scaling) and the most wide spread simulation methods used also in our study of surface growth phenomena. In Chapter 3 we summarize our results concerning the

two main research approaches we applied. The Appendix contains a short description of our Fractal Growth Software [6] which was the first educational software of its kind.

Chapter 2

Theoretical Background

2.1 Mathematical foundations

Here we review very briefly the basic mathematical ideas and notations concerning fractals used in our physical applications. We introduce fractal functions and include some propositions (together with their proofs) based on the works of Falconer [1] and Mandelbrot [2]. Graphs of such functions are generally fractal sets.

2.1.1 Fractals and fractal dimension

We generally work in n-dimensional Euclidean space, $\mathbb{R}^n$. We use the usual Euclidean distance or metric on $\mathbb{R}^n$. If x, y are points of $\mathbb{R}^n$ ($x = (x_1, ..., x_n)$, $y = (y_1, ..., y_n)$) the distance between them can be defined as $|x - y| = (\sum_{i=1}^{n} |x_i - y_i|^2)^{1/2}$.

According to Falconer [1] it seems best to regard a set F as a *fractal* if it has some of the following properties.

- F has a fine structure, i.e., details on arbitrary small scales.
- F is too irregular to be described in traditional geometrical language, both locally and globally.
- Often F has some form of self-similarity, perhaps approximate or statistical.

Figure 2.1: Construction of the middle third Cantor set F, by repeated removal of the middle third of intervals. Note that F_L and F_R, the left and right parts of F, are copies of F scaled by a factor $1/3$

- Usually, the 'fractal dimension' of F (defined in some way) is greater than its topological dimension.
- In most cases of interest F is defined in a very simple way, perhaps recursively.

A well-known fractal is the middle third Cantor set F (Figure 2.1). Although F is quite a large set (uncountable infinite), its size is not quantified by the usual measures such as length — by any reasonable definition F has length zero.

Of the wide variety of fractal dimensions in use, the definition by Hausdorff is the oldest. Hausdorff dimension based on measures can be defined for any set. However, in many cases it is hard to calculate or to estimate it by computational methods. In our physical applications we prefer some more practical definitions.

Let $\dim F$ denote the dimension of F. Fundamental to most definitions of dimension is the idea of 'measurement at scale δ'. For each δ, we measure a set in a way that ignores irregularities of size less than δ, and we see how these measurements behave as $\delta \to 0$. Some typical properties of a 'dimension' are the followings.

Open sets. If F is an open subset of $\mathbb{R}^n$ then $\dim F = n$.

Smooth manifolds. If F is a smooth m-dimensional manifold $\dim F = m$.

Monotonicity. If $E \subset F$ then $\dim E \leq \dim F$.

Stability. $\dim(E \cup F) = \max(\dim E, \dim F)$.

Geometric invariance. If f is a transformation of $\mathbb{R}^n$ such as translation, rotation, similarity or affinity then $\dim f(F) = \dim F$.

For a fractal set F the *box-counting dimension* can be defined as

$$\dim_B F = \lim_{\delta \to 0} \frac{\log N_\delta(F)}{-\log \delta}, \tag{2.1}$$

if this limit exists, where $N_\delta(f)$ is any of the following equivalent definitions:

(i) the smallest number of closed balls of radius δ that cover F;

(ii) the smallest number of cubes of side δ that cover F;

(iii) the number of δ-mesh cubes that intersect F;

(iv) the smallest number of sets of diameter at most δ that cover F;

(v) the largest number of disjoint balls of radius δ with centres in F.

The *lower* and *upper box-counting dimensions* of F are respectively defined if we use $\underline{\lim}$ or $\overline{\lim}$ in (2.1).

Remark 1. *(On the comparison of the box-counting dimension to the classical one). It can be shown that the above mentioned general properties of dimension are fulfilled for the box-counting dimension* $\dim_B F$ *[1]. However, for finite or countable sets* F *resp.* F_i, $\dim_B F \neq 0$ *and* $\dim_B(\cup_{i=1}^{\infty} F_i) \neq \sup_{1 \leq i \leq \infty} \dim_B F_i$ *either, while for such sets the equality would be natural in the case of a classical dimension definition.*

Example. It is easy to show that the box dimension of the middle third Cantor set is $\underline{\dim}_B F = \overline{\dim}_B F = \log 2 / \log 3$.

For most fractals obvious upper estimates of dimension may be obtained using natural coverings by small sets. For the box-counting dimension the following proposition is an immediate consequence of the definitions.

Proposition 1. *Suppose* F *can be covered by* n_k *sets of diameter at most* δ_k *with* $\delta_k \to 0$ *as* $k \to \infty$. *Then*

$$\underline{\dim}_B F \leq \underline{\lim}_{k \to \infty} \frac{\log n_k}{-\log \delta_k}$$

and, if $\delta_{k+1} \geq c\delta_k$ *for some* $0 < c < 1$,

$$\overline{\dim}_B F \leq \overline{\lim}_{k \to \infty} \frac{\log n_k}{-\log \delta_k}.$$

2.1.2 Graphs of functions and fractal functions

A variety of interesting fractals occurs as graphs of functions. Indeed many phenomena display fractal features, e.g., when plotted as function of time.

A function $f : X \to Y$ $(X, Y \subset \mathbb{R}^n)$ is called a *Hölder function of exponent* α if

$$|f(x) - f(z)| \leq c|x - z|^\alpha \qquad (x, z \in X) \tag{2.2}$$

for some constants $c > 0$ and $\alpha > 0$ is the Hölder exponent.

Under certain circumstances the graph of the function $f : [a, b] \to \mathbb{R}$

$$\text{graph} f = \{(t, f(t)) : a \leq t \leq b\}$$

regarded as a subset of the (t, x) — coordinate plane may be a fractal. If f has the continuous derivative or f is of bounded variation, then it is not difficult to see that graph f has dimension 1. However, it is possible for a continuous function to be sufficiently irregular to have a graph of dimension strictly greater than 1. The best known example is the *Weierstrass function*

$$f(t) = \sum_{k=1}^{\infty} \lambda^{(s-2)k} \sin(\lambda^k t) \tag{2.3}$$

where $1 < s < 2$ and $\lambda > 1$. It is a continuous function that is nowhere differentiable and has box dimension s, as we shall see later. Various cases of the Weierstrass function are shown in Figure 2.2.

For a given function f and an interval $[t_1, t_2]$ let

$$R_f[t_1, t_2] = \sup_{t_1 < t, u < t_2} |f(t) - f(u)|$$

denote the maximum range of f over an interval.

Proposition 2. *Let $f : [0, 1] \to \mathbb{R}$ be continuous. Suppose that $0 < \delta < 1$, and m is the least integer greater than or equal to $1/\delta$. If N_δ is the number of squares of the δ-mesh that intersect* graph$f$*, then*

$$\delta^{-1} \sum_{i=0}^{m-1} R_f[i\delta, (i+1)\delta] \leq N_\delta \leq 2m + \delta^{-1} \sum_{i=0}^{m-1} R_f[i\delta, (i+1)\delta]. \tag{2.4}$$

Proof. The number of mesh squares of side δ in the column above the interval $[i\delta, (i+1)\delta]$ that intersect graph f is at least $R_f[i\delta, (i+1)\delta]/\delta$ and at most $2 + R_f[i\delta, (i+1)\delta]/\delta$ using that f is continuous. Summing over all such intervals gives (2.4). This is illustrated in Figure 2.3. □

Figure 2.2: A typical example of fractal functions. The Weierstrass function (2.3) with $\lambda = 1.5$ and (a) $s = 1.3$, (b) $s = 1.5$

The relation between $\dim_B$ and α, the Hölder exponent of a function, is well-known. We can get it by applying Proposition 2 to functions satisfying a Hölder condition with $0 \leq \alpha \leq 1$ as in the following Corollary.

Corollary 1. *Let $f : [0,1] \to \mathbb{R}$ be a continuous function.*

(a) Suppose

$$|f(t) - f(u)| \leq c|t-u|^{2-s} \qquad (0 \leq t, u \leq 1) \tag{2.5}$$

where $c > 0$ and $1 \leq s \leq 2$. Then $\dim_B \operatorname{graph} f \leq s$. This remains true if (2.5) holds when $|t-u| < \delta$ for some $\delta > 0$.

(b) Suppose that there are numbers $c > 0$, $\delta_0 > 0$ and $1 \leq s < 2$ with the following property: for each $t \in [0,1]$ and $0 < \delta \leq \delta_0$ there exists u such that $|t-u| \leq \delta$ and

$$|f(t) - f(u)| \geq c\delta^{2-s}. \tag{2.6}$$

Then $s \leq \underline{\dim_B} \operatorname{graph} f$.

Figure 2.3: The number of δ-mesh squares in a column above an interval of width δ that intersect graph f is approximately the range of f over that interval divided by δ. Summing these numbers gives estimates for the box dimension of graph f.

Proof. (a) It is immediate from (2.4) that $R_f[t_1, t_2] \leq c|t_1 - t_2|^{2-s}$ for $0 \leq t_1, t_2 \leq 1$. With notation as in Proposition 2, $m < (1 + \delta^{-1})$ so

$$N_\delta \leq (1 + \delta^{-1})(2 + c\delta^{-1}\delta^{2-s}) \leq c_1\delta^{-s}$$

where c_1 is independent of δ. The result now follows from Proposition 2.

(b) In the same way, (2.6) implies that $R_f[t_1, t_2] \geq c|t_1 - t_2|^{2-s}$. Since $\delta^{-1} \leq m$, we have from (2.4) that

$$N_\delta \geq \delta^{-1}\delta^{-1}c\delta^{2-s} = c\delta^{-s}$$

so equivalent definition (iii) of $\dim_B$ gives $s \leq \underline{\dim}_B \, \mathrm{graph} f$. □

In our physical applications we are going to work with *self-affine or fractal functions* [2], $f(x) \in \mathbb{R}$, which are continuous and $\forall \lambda$ have the property

$$f(x) \simeq \lambda^{-\alpha} f(\lambda x), \tag{2.7}$$

where $\alpha > 0$ is some constant exponent.

(2.7) expresses the fact that the function is invariant under the following *anisotropic — direction dependent rescaling*: shrinking along the x axis by a factor of $1/\lambda$, followed by rescaling of the values of the function (measured in the perpendicular direction) by a different factor $\lambda^{-\alpha}$. For some deterministic self-affine functions this can be done exactly, while for random functions the

above considerations are valid only in stochastic sense (expressed by using the sign $\simeq$).

A rough interface (occuring in growth phenomena as we shall see in 2.2) can be well described in terms of such fractal functions.

Remark 2. *Self-affine functions, $f : [0,1] \to \mathbb{R}$, are locally Hölder functions satisfying (2.2) with Hölder exponent $0 \leq \alpha \leq 1$ (see, e.g,[2]). Then according to Corollary 1, provided λ is large enough, their local fractal dimension is $\dim_B \text{graph} f = s$ where $1 < s < 2$.*

Example of a typical self-affine function is the Weierstrass function defined by (2.3). Suppose $\lambda > 1$ and $1 < s < 2$. It is easy to see that first derivative of the above function diverges everywhere, although the function itself is continuous. Formally replacing k with $k+1$ we get the scaling relation $f(t) = \lambda^{-(2-s)} f(\lambda t)$.

Calculation of the local dimension of Weierstrass functions. Given $0 < h < 1$, let N be the integer such that

$$\lambda^{-(N+1)} \leq h < \lambda^{-N}. \tag{2.8}$$

Then

$$|f(t+h) - f(t)| \leq \sum_{k=1}^{N} \lambda^{(s-2)k} |\sin(\lambda^k(t+h)) - \sin(\lambda^k(t))|$$

$$+ \sum_{k=N+1}^{\infty} \lambda^{(s-2)k} |\sin(\lambda^k(t+h)) - \sin(\lambda^k(t))| \leq \sum_{k=1}^{N} \lambda^{(s-2)k} \lambda^k h + \sum_{k=N+1}^{\infty} 2\lambda^{(s-2)k}$$

using the mean-value theorem on the first N terms of the sum, and an obvious estimate on the remainder. Summing these geometric series,

$$|f(t+h) - f(t)| \leq \frac{h\lambda^{(s-1)N}}{1-\lambda^{1-s}} + \frac{2\lambda^{(s-2)(N+1)}}{1-\lambda^{s-2}} \leq ch^{2-s}$$

where c is independent of h. Then using (2.8) Corollary 1(a) now gives $\overline{\dim}_B \text{graph} f \leq s$.

In a similar way, but splitting the sum into three parts — the first $N-1$ terms, the Nth term, and the rest — if (2.8) holds we get

$$|f(t+h) - f(t) - \lambda^{(s-2)N}(\sin(\lambda^N(t+h)) - \sin(\lambda^N t))| \leq \frac{\lambda^{(s-2)N-s+1}}{1-\lambda^{1-s}} + \frac{2\lambda^{(s-2)(N+1)}}{1-\lambda^{s-2}}. \tag{2.9}$$

Suppose $\lambda > 2$ is large enough for the right-hand side of (2.9) to be less than $\frac{1}{20}\lambda^{(s-2)N}$ for all N. For $\delta < \lambda^{-1}$, take N such that $\lambda^{-N} \leq \delta < \lambda^{-(N-1)}$. For each t we may choose h with $\lambda^{-(N+1)} \leq h < \lambda^{-N}$ such that $|\sin \lambda^N(t+h) - \sin \lambda^N t| > \frac{1}{10}$, so by (2.9)

$$|f(t+h) - f(t)| \geq \frac{1}{20}\lambda^{(s-2)N} \geq \frac{1}{20}\lambda^{(s-2)}\delta^{2-s}.$$

It follows from Corollary 1 (b) that $\underline{\dim}_B$ graph$f \geq s$.

The Weierstrass function is representative of a more general class, i.e. if g is a suitable periodic function, a similar method for the calculation of the dimension applies. Namely

$$f(t) = \sum_{k=1}^{\infty} \lambda^{(s-2)k} g(\lambda^k t)$$

has $\dim_B$ graph$f = s$. Such functions may occur in dynamical systems [1].

2.1.3 Power-law behaviour of fractal functions

One way in which the fractal nature of a graph of a function is often manifested is by a power-law behaviour of the correlation between measurements separated by time h. In this section we only outline the ideas involved [1]; without being rigorous. In particular, the limits are all assumed to exist.

For convenience of analysis, we assume that $f : (-\infty, \infty) \to \mathbb{R}$ is a continuous bounded function and we consider the average behaviour of f over long periods $[-T, T]$. Similar ideas hold if f is just defined on $[0, \infty)$, or on a finite interval, by extending f to $\mathbb{R}$ in a periodic manner. We write $\overline{f}$ for the average value of f, i.e.

$$\overline{f} = \lim_{T\to\infty} \frac{1}{2T} \int_{-T}^{T} f(t)dt.$$

A measure of the correlation between f at times separated by h is provided by the *autocorrelation function*

$$C(h) = \lim_{T\to\infty} \frac{1}{2T} \int_{-T}^{T} f(t+h)f(t)dt - (\overline{f})^2.$$

Since

$$\int (f(t+h)-f(t))^2 dt = \int f(t+h)^2 dt + \int f(t)^2 dt - 2\int f(t+h)f(t)dt$$

we have

$$\begin{aligned} C(h) &= (\overline{f})^2 - \overline{f^2} - \tfrac{1}{2}\lim_{T\to\infty} \tfrac{1}{2T}\int_{-T}^{T}(f(t+h)-f(t))^2 dt \\ &= C(0) - \tfrac{1}{2}\lim_{T\to\infty} \tfrac{1}{2T}\int_{-T}^{T}(f(t+h)-f(t))^2 dt \end{aligned}$$

where

$$\overline{f^2} = \lim_{T\to\infty} \frac{1}{2T}\int_{-T}^{T} f(t)^2 dt$$

is the mean square of f, assumed to be positive and finite. Now we use Corollary 1 to show the relationship between the autocorrelation function of f and the dimension of graph f. Suppose that f is a function satisfying (2.5) and also satisfying (2.6) in a reasonable uniform way. Then there are constants c_1 and c_2 such that

$$c_1 h^{4-2s} \le \frac{1}{2T}\int_{-T}^{T}(f(t+h)-f(t))^2 dt \le c_2 h^{4-2s}$$

for small h. While it is not directly equivalent to (2.5) and (2.6) in many reasonable time-homogeneous situations, the conditions do correspond. Thus if the autocorrelation function of f satisfies

$$C(0) - C(h) \simeq c h^{4-2s} \tag{2.10}$$

for small h we can expect the box dimension of graph f to be s.

Autocorrelations provide us with several methods of estimating the dimension of the graph of a function f. If the power law behaviour (2.10) is observed for small h then

$$\dim_B \text{ graph} f = 2 - \lim_{h\to 0} \frac{\log(C(0)-C(h))}{2\log h}$$

if this limit exists.

2.2 Physical background — Surface growth

Solids form through growth processes which take place at the surface. If the conditions of the growth process are such that the development of the interface is marginally stable and the fluctuations are relevant, the resulting structure is a rough surface and can be well described quite often by a formalism based on the concept of scale invariance and on self-affine *fractal functions*. Marginal stability means that the fluctuations (which die out quickly for a stable surface and grow exponentially for an unstable one) survive without drastic changes for a long time. In many cases the growth and roughening of a surface advances as new parts are added according to some dynamical process.

In the following part we review the surface growth phenomena [5], [11], [4] related to our results using the notations widespread in the physics literature. The dynamics of fractal surfaces is described at first by the help of scaling theory, then by some simple lattice models of simulating growth. We briefly present the different types of related continuum equations together with the general ideas concerning their numerical solution. In most cases we shall work with the time and one space variable, considering space as $1+1$-dimensional one.

2.2.1 Dynamic scaling

Dynamic roughening of interfaces is an example of a far-from-equilibrium phenomenon. The analysis of the scaling behaviour of the time and spatial dependence of the surface properties has led to the development of a general dynamic scaling approach for describing growing interfaces. During the growth of compact (non-fractal) objects the motion of the interface is directed outward, and this orientation plays a special role. Typically, the interface can be well approximated by a single valued function of $d-1$ variables, e.g. one can describe the properties of the surface by examining only those points of the object which are farthest from the centre of the structure in a given direction. The scaling properties of such surfaces are direction dependent (anisotropic): parts of various sizes can be rescaled into an object with the same overall behaviour using a rescaling factor in the direction parallel to the growth which is different from that needed to rescale the perpendicular lengths.

The evolution of interfaces is generally governed by stochastic processes involving nonequilibrium many-body effects. These complexities preclude applications of standard analytical approaches to this problem. On the other hand, it has been recognized that growing surfaces are fractal and naturally evolve to a steady-state having no characteristic time or length scale which led to the development of the scaling theory for describing the dynamics of fractal surfaces. In 1985 a dynamic scaling formalism based on the surface width was introduced providing a tool for both theoretical and experimental studies of surfaces [9]. It has several alternative — but completely equivalent — forms. Here we use the original formulation.

We consider the time evolution of a rough interface in a d-dimensional space starting from an initially flat surface at time $t = 0$. In particular, let us concentrate on a part of the surface having an extent L in $d-1$-dimensions perpendicular to the growth direction. The growing surface typically can be described by a single-valued function $h(r,t)$ which gives the height (distance) of the interface at position r (along the substrate) at time t measured from the original $d-1$ dimensional flat surface. In the cases where the surface cannot be described by a single valued function of r, we assume that the function $h(r,t)$ corresponds to the maximum height of the surface at r. During growth the interface heights fluctuate about their average value and the extent of these fluctuations characterizes the width or the thickness of the interface. The root mean-square of the height fluctuations $w(r,t)$ is a quantitative measure of the *surface width* and is defined by

$$w(r,t) = [\langle h^2(r,t)\rangle_r - \langle h(r,t)\rangle_r^2]^{1/2}. \tag{2.11}$$

Thus, the width $w(L,t)$ is a measure of the correlations along the direction of growth and perpendicular to the $d-1$ directions along the surface. Here $\langle\ \rangle_r$ denotes the spatial average taken by space variable r at fixed time t. Since we assume that the surface is a continuous function, its width has to saturate to some value after some relaxation time τ. The only scale in the problem is the linear size of the substrate r (there is no size independent time scale), thus, w depends only on some power of r and a ratio of the form t/r^z, where z is an exponent describing how the relaxation time depends on the system size.

Correspondingly, the *dynamic scaling* of the surface width has the form

$$w(r,t) = r^{\alpha} f(t/r^{\alpha/\beta}), \tag{2.12}$$

where $\alpha/\beta = z$ is the *dynamic scaling exponent.*

In the limit where the argument of the scaling function $f(y)$ is small, $y \ll 1$, the width depends only on t and this implies that for small y the scaling function $f(y)$ has to be of the form $f(y) \sim y^{\beta}$. Saturation at large times means that $f(y)$ goes to a constant in that limit and the surface reaches a steady-state characterized by a constant value of the width. The surface is scale invariant and becomes a self-affine fractal function with Hölder exponent α. In physics α is often referred to as roughness exponent, while Mandelbrot called it Hurst exponent at first. From the above it follows that for long times and $r < L$

$$w(r, t \to \infty) \sim r^{\alpha}, \tag{2.13}$$

and for fixed r (e.g., $r = L$) and short times

$$w(r, t) \sim t^{\beta}. \tag{2.14}$$

An alternative approach to the characterization of self-affine surfaces changing in time is the determination of various correlation functions. One of the most convenient quantities is the *height-height correlation function* $c(r, t)$ defined as

$$c(r, t) = \langle |h(r', t') - h(r' + r, t' + t)| \rangle_{r', t'},$$

which is the average height difference measured for a time difference t at two points whose coordinates on the substrate are separated by r. On the basis of the scaling behaviour of self-affine functions, $c(r, t)$ scales the same way as the width,

$$c(r, t) = r^{\alpha} f_1(t/r^{\alpha/\beta}), \tag{2.15}$$

with a scaling function $f_1(x)$ analogous to the above described one.

For the surfaces obtained experimentally or numerically from a growth model the expressions (2.13) and (2.14) can be used to determine the exponents α and β. In these formulas instead of $w(r, t)$ often the averaging of surface width over samples (e.g. many simulation runs or many experiments) is considered. In most cases the exponents α and β are effectively derived from the log-log plot of the corresponding quantities (using the surface width or some appropriate correlation function).

In their turn these exponents provide us with a quantitative tool for analyzing the microscopically different stochastic growth models. The scaling exponents define some universality classes, so the different models with the same exponents belong to the same universality class. Most of the studies of

self-affine growth concentrate on the determination of the exponents α and β characterizing the time development of surfaces.

2.2.2 Lattice models of surface growth

One of the most successful approaches to understanding the dynamics of growing interfaces has been the study of simplified numerical models or phenomenological equations capturing the essential physics of a given growth process.

At first let us consider the most typical lattice models simulating aggregation of particles and stochastic surface growth (see, e.g., our paper [32]).

Structures consisting of connected particles are usually called *clusters* or *aggregates*. In most of the cases the growth will be assumed to take place on a *lattice* for computational convenience, and two particles are regarded as connected if they occupy nearest neighbour sites of the lattice. A lattice site with a particle assigned to it is called *occupied* or *filled*. An important additional feature included into the majority of models to be described is stochasticity which is typical for growth phenomena.

In general, a stochastic cluster growth model may lead to all possible configurations which can be formed from a given number of particles. What makes these models differ from each other is the weight or probability $P_{L,i}$ associated with a given configuration i consisting of N units. $P_{L,i}$ can be different for the same configuration even in the same model, because generally it depends on the sequence, according to which the individual particles are added to the cluster.

There are two main types of cluster growth processes, depending on the global character of the rule which is used in the course of adding a particle (or a cluster of particles) to the growing cluster. *The rule will be called local if it depends only on the immediate environment* of the position where the new particle is to be added. In other words, when deciding whether to add a particle at site $\vec{\mathbf{x}}$ only the status (filled or not) of the nearest or next nearest neighbours of this site is taken into account. On the contrary, *in non-local models the structure of the whole cluster* can affect the probability of adding a site at a given position. In the following we deal with local models related to our continuum equations. There are two typical geometries considered in the simulations of fractal aggregation. In the first case the growth starts from a

Figure 2.4: Lattice models of surface growth created by the Fractal Growth program package ([6]). (a) Eden model in a strip. (b) Ballistic deposition

single particle and usually results in isotropic aggregates, while in the second geometry the initial configuration is assumed to be a hyperplane (chain, a two dimensional lattice, etc. of seed particles). If the growth starts along a plane, the object we investigate is the advancing and gradually roughening surface of the growing structure. This surface is usually anisotropic and can be described in terms of self-affine fractals.

The two most studied aggregation models leading to self-affine surfaces are the Eden and the ballistic aggregation models. There is a rich variety of different modifications of these models in the literature, however, all of them have the same dynamic scaling properties. The algorithms considered here are implemented on a square lattice of horizontal width L, with periodic boundary conditions imposed in the lateral directions, and of infinite vertical extent.

(i) *Eden model.* (Figure 2.4a) A row of seed particles is placed at the base and a cluster is grown by randomly choosing one of the empty sites next to the aggregate (perimeter sites). In the simulations of the most common version of the Eden model a single perimeter site is filled with probability $1/N(p)$ where $N(p)$ is the total number of perimeter sites. Therefore, each nearest neighbour site to the cluster has the same probability to be occupied at the given time step. A large cluster is obtained after having repeated this procedure many times.

It is well-known (see,e.g., [10]) that the width of the simulated surface grows as the cubic root of the time and saturates at a value which is proportional to the square root of L. This fact expresses the dynamic scaling of our self-affine surface, namely $\alpha = 1/2$ and $\beta = 1/3$.

(ii) *Ballistic deposition.* (Figure 2.4b) Here, a column $i \in \{1, ..., L\}$ is picked at random, a particle is dropped vertically in that column and sticks upon first contact with the evolving deposit. The update rule is:

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

where the surface position h and space coordinate i assume integer values. Here $h(i, t+1)$ denotes the height at the new time level $t+1$, which is computed from the corresponding height values at the previous time level t. After many iterations, it produces a highly non-trivial structure e.g, the sizes of the empty regions are widely scattered. In spite of this, the structure can be considered homogeneous on a large length scale and its average height grows linearly with time. But more importantly, the deposit has a rough surface which can be shown to be a self-affine fractal. Extensive simulations indicate that in the asymptotic limit the structure of the surface is such that its vertical extension (width) is equal to the square root of its horizontal size [9], ($\alpha = 1/2$). This is precisely what self-affinity means.

Both models lead to surfaces exhibiting interesting scaling both in space and time corresponding to the dynamic scaling principle. By going to very large length and time scales they are truly described by the same exponents, indicating that they belong to the same universality class. The introduced models and their different versions can easily be programmed and are contained in our Fractal Growth software package [6] including other growth models as well (see briefly in the Appendix).

2.2.3 Stochastic differential equations for surface growth

There were several attempts to construct a continuum equation for describing the dynamics of growing surfaces.

Equilibrium surface growth is often modelled by the Langevin equation which describes how a surface relates under the balance of a driving noise term due to relaxation mechanisms such as surface tension or diffusion. For

far from equilibrium models, we are interested in, also a Langevin type equation of motion is suggested. Let us denote by h the local height of the surface above a d-dimensional substrate corresponding to growth in a $(d+1)$-dimensional space. It is convenient to ignore overhangs so that h can be considered as a single valued function of $x \in \mathbb{R}^d$. Therefore one can assume that local coarse scale derivatives $\partial h/\partial x$ exist. Let us now express the velocity of the interface $h(x,t)$ as a function of its local gradient. To take into account the stochastic nature of the growth we can write down the simplest nonlinear Langevin equation for $\tilde{h} = h - vt$ (v is the velocity normal to the surface). In 1982 Edwards and Wilkinson [3] derived a continuum partial differential equation (PDE) of this type – *EW equation* – for describing the growth of an interface

$$\frac{\partial h}{\partial t} = \nu \nabla^2 h + \eta(x,t) \tag{2.16}$$

where the time variable t is associated with the average deposition height $\overline{h}$ and ν is a constant (related to the surface tension). $\eta(x,t)$ is assumed to have a Gaussian distribution with zero-mean, e.g., such that

$$\langle \eta(x,t)\eta(x',t') \rangle = 2D\delta(x-x')\delta(t-t'), \tag{2.17}$$

so it would be an uncorrelated noise term. Here $D > 0$ is a constant and $\delta(x)$ is the well-known delta function.

The first term in (2.16) describes the relaxation of the interface due to the surface tension ν. Its meaning is quite obvious; protrusions (places with local curvature $\nabla^2 h < 0$) tend to disappear under the influence of the smoothing effect of surface tension. η is included to take into account the fluctuations: the process of random deposition. Equation (2.16) provides a phenomenological description for the type of ballistic deposition processes described earlier. In 1986 Kardar, Parisi and Zhang (KPZ) extended the EW equation [13]. In order to take into account the sideways growth in the ballistic aggregation and Eden models they proposed an additional nonlinear term which is the lowest-order non-vanishing term in a gradient expansion. In general the growth takes place in a direction locally normal to the interface. When a particle is added, the increment projected onto the h axis (as it is shown in Figure 2.5) is $\delta h = [(v\delta t)^2 + (v\delta t \nabla h)^2]^{1/2}$ which leads in the weak gradient limit to

$$\frac{\partial h}{\partial t} = v[1 + (\nabla h)^2]^{1/2} \simeq v + (v/2)(\nabla h)^2 + ... \tag{2.18}$$

Figure 2.5: Schematic picture showing the increment of h as the growth locally occurs along the normal to the interface

The above expression reduces to $\lambda/2(\nabla h)^2$ after transformation to the co-moving frame (like in (2.16)). Here λ is a constant. Then the *KPZ equation* reads

$$\frac{\partial h}{\partial t} = \nu_0 \nabla^2 h + \lambda/2(\nabla h)^2 + \eta(x,t), \tag{2.19}$$

ν_0 is a constant related to the surface tension,η is a noise term, in the original version it is an uncorrelated Gaussian noise term with zero-mean as (2.17).

The KPZ equation (2.19) enjoys a subtle local symmetry: Galilean invariance. This symmetry has its origin in the fact that if we tilt the mathematical coordinate system slightly by an infinitesimal angle ε, our dynamical equation should remain invariant, since the physics remains manifestly so. If we apply the following coordinate transformation to our equation

$$h \to h + \varepsilon\ x, \qquad x\ \to x + \lambda\varepsilon t$$

then it leaves our equation invariant. As a consequence of this local symmetry there is a characteristic identity between the two fundamental scaling exponents, (the roughness or Hölder exponent and the dynamic scaling exponent)

$$\alpha + z = 2 \tag{2.20}$$

which is called *KPZ scaling relation* [14].

The KPZ equation (2.19) embodies three different universality classes, depending on the values of the parameters ν_0 and λ.

(i) The $\nu_0 = 0$, $\lambda = 0$ case corresponds to random deposition of particles without surface restructuring or sticking of the particles to each other. Then for $L \gg 1$ the columns grow according to the Poisson statistics describing the probability that the number of particles in a given column is equal to h if $\overline{h}$ particles per column have been deposited. Thus $w \sim \overline{h}^{1/2}$ is given by the central limit theorem, and $\beta = 1/2$. Since the size of the substrate does not have an effect on w, the other two exponents can be regarded to be equal to zero.

(ii) If $\lambda = 0$, it corresponds to the linear EW equation (2.16) when the evolution of the interface is dominated by the surface restructuring. For this case $\alpha = (3-d)/2$, $\beta = (3-d)/4$ and $z = 2$ as it can be obtained by Fourier transforming the equation [3]. We expect that the large scale behaviour of the growth model is again governed by the dynamic scaling theory. Since equation (2.16) is linear, it is easy to solve it by Fourier methods. The surface width of the fluctuating interface can be computed $w^2(L,t) = \langle L^{-d-1} \int_0^L d^{d-1}x[h(x,t) - \overline{h}]^2 \rangle$ where the angular brackets denote the averaging over samples and $\overline{h}$ is the mean height. Direct integration shows for w the following scaling behaviour

$$w^2(L,t) \sim \frac{D}{\nu_0} L^{\alpha} f_{EW}(\nu t / L^2)$$

where $\alpha = (3-d)/2$ and

$$f_{EW}(x) = \frac{K_d}{(3-d)(2\pi)^{3-d}} (1 - e^{-8\pi^2 x + (8\pi^2)^{(3-d)/2}} \int_{8\pi^2}^{\infty} y^{(3-d)/2} e^{-y} dy)$$

with $K_d = 2^{d-2}\pi^{(d-1)/2}\Gamma((d-1)/2)$. We can get $\beta = (3-d)/4$ and $z = 2$. It was shown that for $d = 2$ ($(1+1)$ dimension) $\beta = 1/4$, $\alpha = 1/2$.

(iii) The third universality class corresponds to the general case when neither ν_0 nor λ is equal to zero. Here the following exponents were found $\alpha = (3-d)/2$, $\beta = (3-d)/3$ and $z = 3/2$.

The KPZ equation has been thoroughly analyzed for one-dimensional interfaces [13]. In case when the nonlinear term λ vanishes it corresponds to EW equation with scaling exponents as indicated above. For large λ it gives $\beta = 1/3$, $\alpha = 1/2$ and $z = 3/2$. Simulations of various surface growth models like, e.g., Eden or ballistic deposition are in good agreement with

these values, implying that the KPZ equation provides a proper description of surface evolution in this class of growth processes.

The KPZ universality class describes most of the physically relevant and important cases of non-equilibrium surface growth. In KPZ class further investigations were motivated for e.g. by the fundamental question: what features are responsible dictating the universality class of a particular roughening process.

2.2.4 Deterministic differential equations for surface growth

As was shown by Kardar, Parisi and Zhang a relatively simple nonlinear partial differential equation with a stochastic term could successfully be used to describe the major features of the process of roughening in a wide class of surface growth phenomena [13]. Under some conditions, however, the appearently stochastic development of the interface is not due to an external noise, but is a result of an underlying instability. Thus, a possible alternative description of rough surface growth can be based on simple *deterministic partial differential equations containing a singular or unstable term.* A well-known example of this type, the Kuramoto-Sivashinsky (KS) equation ($\partial h/\partial t = -\nabla^2 h + |\nabla h|^2 - \Delta^4 h$), has been argued to describe the propagation of flame fronts. The simultaneous effects of the unstable, nonlinear and the stabilizing terms in the KS equation have been shown to result in a chaotic spatiotemporal behaviour of the solutions being fractally rough (self-affine) on large length scales [24].

In an interesting approach to d dimensional complex spatio-temporal behaviour the various functions associated with these structures are considered as growing rough surfaces in a $d+1$ dimensional space [25]. This development connects the studies of growing fractal surfaces to the research how stochastic spatio-temporal behaviour emerges in more complex deterministic processes.

In the following we shall consider perhaps the simplest family of deterministic PDE-s producing growing fractal surfaces. These equations, originally proposed by Zhang have the form

$$\frac{\partial h(x,t)}{\partial t} = \nabla^2 h(x,t) + \text{singular term} \tag{2.21}$$

where several forms of the singular term can be used, including

$$|\nabla h|^{\alpha} \qquad \text{with} \qquad \alpha < 1 \tag{2.22}$$

or

$$\ln(|\nabla h|). \tag{2.23}$$

Zhang argued that the complex directed polymer problem leads to an equation analogous to (2.21). Here we simply assume that the simultaneous effects of more complicated mechanisms under some conditions can be accounted for by a simple singular term of the form we are considering. The time dependence of the roughness W of surfaces generated by (2.21) with (2.23) was investigated by Zhang who found that $W \sim t^{\beta}$ with $\beta \simeq 0.2$.

It was Zhang who recently proposed that the above equation for $\alpha < 1$ is expected to produce chaotic behaviour. He showed that the singular term results in an instability for $0 < \alpha < 1$; small perturbations would grow exponentially and they become tamed only by the Laplacian term. Following Zhang's suggestion, Amar and Family ([18]) numerically integrated Eq. (2.21) with (2.22) for $\alpha = 1/2$. In this case (2.22) does not diverge as $\nabla h \to 0$, however, the corresponding term is unstable (we shall consider later on the case with singular terms diverging as $\nabla h \to 0$). They determined β and the Lyapunov exponents corresponding to the chaotic behaviour of (2.21) with (2.22). They also observed a grooved phase characterized by occasionally occuring and disappearing linear parts embedded into the rough interface.

Neither version of the equation of Zhang are well understood mathematically in spite of their simple form. Nothing is known about the existence, uniqueness and stability of solutions. For (2.21) with (2.23) only the solutions with non-empty set of extremal singular points, where $u_x = 0$, are of physical interest. We shall investigate the numerical and analytical solutions of both types of the above mentioned singular interface equations.

2.2.5 Numerical solution of surface growth equations

The surface growth equations are solved numerically. We show here the most often used numerical method — a standard finite difference algorithm [20]. We briefly review it for the KPZ type equations (2.19) with initial value $h(x, 0) = 0$ in $1 + 1$ dimension.

Let us introduce a grid of mesh points $(x,t) = (i\Delta x, j\Delta t)$. Here $\Delta x, \Delta t$ are the mesh parameters which are small (and thought of tending to zero), and i, j are integers, $j > 0$, $i = 1, 2, ..., L$, $L > 1$ is a constant (we work with finite linear size in x direction). We then look for an approximate solution of (2.19) at these mesh points. We need some boundary conditions in x direction: because of physical considerations either we may use (i) *free boundary conditions* $h(0,t) = h(1,t)$ and $h(L+1,t) = h(L,t)$ or (ii) *periodic boundary conditions* $h(0,t) = h(L,t)$ and $h(L+1,t) = h(1,t)$. The spatial derivatives of the right hand side of (2.19) are discretized using standard forward-backward differences with the mesh parameter Δx. We integrate (2.19) by using the Euler algorithm with time increments Δt [8]. Then the discretized equation is

$$\begin{aligned} h(x,t+\Delta t) &= h(x,t) + \frac{\Delta t}{(\Delta x)^2}((h(x+\Delta x,t) - 2(x,t) + h(x-\Delta x,t)) \\ &\quad + \frac{1}{8}\lambda(h(x+\Delta x,t) - h(x-\Delta x,t))^2) + \text{discr. noise.} \quad (2.24) \end{aligned}$$

The *discretization of the noise term* depends on the type of the noise we are using. For the *stochastic noise* when η is an uncorrelated Gaussian noise term with zero-mean, namely $\langle \eta(x,t)\eta(x',t')\rangle = 2D\delta(x-x')\delta(t-t')$, ($D > 0$ is a constant), we can take the discretization $\eta(\Delta x, \Delta t) = \sigma\sqrt{12\Delta t}R(t)$. Here $\sigma^2 = 2D/(\Delta x)^2$ and random numbers R are uniformly distributed between $-1/2$ and $1/2$. The prefactor $\sigma\sqrt{12\Delta t}$ guarantees that the noise has the same second moment as the Gaussian noise integrated over the time interval Δt (see, e.g., [7]).

In the *quenched noise* case $\eta(x,h)$ depends on the surface $h(x,t)$ in a highly nonlinear way. Usually we suppose that $\langle \eta(x,h)\rangle = 0$ and η is an uncorrelated quenched noise with Gaussian distribution of amplitudes and a correlator which in the continuum limit is formally given by

$$\langle \eta(x_0,h_0)\eta(x_0+x', h_0+h')\rangle = D\delta(x')\delta(h')$$

($D > 0$ is a constant). Then we define the discretized noise on a two dimensional lattice: we put $\eta(x,[h(x,t)])$ into (2.24) where $[h(x,t)]$ denotes integer part (see [19]), and η is chosen to be uniformly distributed on the interval $(0,1)$. Then the noise is correlated over the distance of a lattice spacing.

The discretization parameters Δx and Δt have to be chosen small enough to ensure the stability of the algorithm. For the deterministic linear equation ($\lambda = 0, D = 0$) in (2.19), a simple von Neumann stability (see e.g.,[8])

analysis gives the condition $\Delta t < \Delta x^2/2$. Above this limit even the discretized Laplacian in (2.24) would be numerically unstable. Empirically it was found that Δt has to be significantly smaller than this upper bound for the nonlinear stochastic equation, so the stability limit no longer increases like Δx^2 but with a smaller power. In fact a scaling analysis suggests that $\Delta t <$ constans $(\Delta \mathrm{x})^{\mathrm{z}}$ should be required (where z is the scaling exponent). By physical considerations $\Delta x = 1$ is used in most of the simulations.

For the numerical solution of the singular interface equations (2.21) with (2.23) or (2.22) we shall use also the simple finite difference method and similar reasoning for the choices of stepsizes Δx, Δt.

Chapter 3

Results

3.1 Simulations of surface growth related to physical experiments

By the beginning of the 1990 years a considerable amount of interesting results has accumulated about the far from equilibrium growth of fractal surfaces as we could see in 2.2. From the available data it became clear that perhaps the most exciting question regarding the growth of rough interfaces was the apparent discrepancy between the experimental results and the corresponding predictions based on the most general theoretical approaches and related simulations. In particular, in the $1+1$ dimensional case of KPZ for the exponents describing the dynamic scaling of the width of the surface $\alpha = 1/2$ and $\beta = 1/3$ were predicted.

On the other hand, the existing experimental estimates obtained for the interface of viscous flows and the surface of bacteria colonies range between 0.63 and 0.81 for α and give $\beta \simeq 0.65$. These values are in clear conflict with the predictions 1/2 and 1/3. There are many more experimental systems in which the measured roughness exponents differ from the KPZ values.

During the past decade a few specific models have been proposed to eliminate the above mentioned disagreement. In some cases the original KPZ equation is modified by adding additional terms to it or in other cases the type of the noise $\eta(x,t)$ is changed.

We worked with different approaches (i) using *multiplicative noise* term instead of the original *additive* one, or (ii) instead of the originally *stochastic noise* term we dealt with *quenched noise* $\eta(x,h)$ which was fixed in space and

depended on the coordinate x, as well as the precise interface position h, but not explicitly on t.

Our goals were (i) to make assumptions which are as close to the experimental conditions as possible, (ii) to numerically investigate the resulting equation and (iii) to compare the obtained behaviour with that observed in the experiments.

In our papers [27],[28] concentrating on the experiments of the advancement of a wetting fluid in inhomogeneous media we introduced a new concept of studying the actual physical situation by considering a stochastic differential equation for the surface development with a multiplicative quenched noise. We argued that multiplicative noise is the appropriate choice to describe experiments where the interface between two flowing phases is considered.

We proposed that the development of the interface $h(x,t)$, e.g., in the experiments on quasi 1+1 dimensional viscous flows is described by the equation

$$\frac{\partial h}{\partial t} = \left(\nabla^2 h + v(1+(\nabla h)^2)^{1/2}\right)(p+\eta), \tag{3.1}$$

where $p > 0$ is some constant, v is the normal velocity of the growing interface and the term $\eta > 0$ corresponds to quenched noise with no correlations, i.e.,

$$\langle \eta(x,h)\eta(x',h')\rangle = C\delta(x-x')\delta(h-h'). \tag{3.2}$$

From physical considerations here we *do not assume* that the distribution of the noise amplitudes is Gaussian with a zero mean; it would be equivalent to supposing that flat parts of the interface would move backward at places with $\eta < -p$. Rather, we shall assume that η follows some other simple distribution, e.g., the uniform distribution. In this way, we can avoid (unlike in the case of Gaussian distribution) the occurrence of the unphysical values $p + \eta < 0$.

To support the particular form in which the noise term enters (3.1) let us consider the experiment on the two phase flow of viscous fluids in porous media. We are interested in the case when the more viscous, wetting fluid advances due to the presence of capillary forces and the interface exhibits kinetic roughening. Under such circumstances the system can be considered as a network of randomly interconnected channels of widely distributed sizes and geometry. The motion of the wetting fluid is determined by the simultaneous effects of surface tension, capillary forces and local flow properties

(permeabilities of the channels). The advancement of the interface at a given point is proportional to the local driving force and the permeability (Darcy's law); just as the electric current $\vec{j}$ is proportional to the conductivity σ and the electric field $\vec{E}$, $\vec{j} = \vec{E}\sigma$. In our case the driving forces are (i) the wetting or capillary force which would produce velocity v for unit permeability and, (ii) the forces due to the surface tension which are represented by the term $\nabla^2 h$ (we assume that there is no extra pressure applied to the penetrating fluid). Thus, equation (3.1) is equivalent to

$$v_s = F\varepsilon, \tag{3.3}$$

where v_s is the velocity of the surface in the vertical direction, ε is the randomly changing local permeability and F denotes a general driving force. Although here we used the wetting experiment as an example to justify the necessity to take into account multiplicative noise, we think that in many other situations (e.g., motion of domain walls in magnetic systems with random fields and pinning of charge density waves) our approach should also be considered.

Next let us make a few relevant comments on the other aspects of the proposed equation (3.1). (i) The term $v(1 + (\nabla h)^2)^{1/2}$ is included in its full form from the gradient expansion (2.18) (instead of its linearized version used in the KPZ equation), because in the actual experiments at the majority of the points along the interface the condition $|\nabla h| \ll 1$ is not satisfied. This statement becomes very relevant when pinning forces are present and the interface develops deep valleys with $|\nabla h| \gg 1$ playing a determining role in the process of roughening. (ii) Naturally, equation (3.1) can be extended by including other terms, e.g, an explicit additive noise ζ which can be independent of or proportional to η, and a term $\lambda(\nabla h)^2$ instead of $(\nabla h)^2$ only (λ is a parameter). In this case (3.1) reads as

$$\frac{\partial h}{\partial t} = \left(\nabla^2 h + v(1 + \lambda(\nabla h)^2)^{1/2}\right)(p + \eta) + \zeta. \tag{3.4}$$

In fact, even without including additive noise explicitly, in (3.1) or in the above equation the term $v(1 + \lambda(\nabla h)^2)^{1/2}\eta$ has a contribution which corresponds to additive noise. If both types of noise are present, one may expect that in the limit of very large system sizes and long times the additive noise will dominate the growth since the various derivatives of the surface become very small on a coarse grained scale. The detailed discussion of this important question cannot be included into the present work. The only feature

we note here is that choosing $\lambda, v \ll 1$ in (3.4) the additive noise can be made arbitrarily small and the behaviour is determined by the multiplicative nature of the noise. This regime then is likely to *cross over* to the additive noise dominated case after arbitrarily long characteristic time.

Now we are in the position to describe the development of the interface in terms of kinetic roughening dominated by pinning forces. At places where $p + \eta \ll 1$, the motion of the interface slows down dramatically. These points can be considered as temporarily pinned. However, like in all of the existing experiments on growth (with no evaporation), after some time the surface passes by this place or region of low permeability and advances further without a complete stop.

An interesting special case of the noise is when η depends only on x. An existing aspect of the physics is reflected by this choice: the motion of the interface is determined not only by the conditions at the surface, but also by the permeability of regions already left behind (which may partially block the supply of additional fluid).

Before describing our numerical studies of (3.1) we briefly discuss the *applicability* of the KPZ approach to the experiments on wetting fronts. According to the KPZ equation the development of the surface is described by (2.19) where λ is a parameter which for wetting flows is larger than 0. As was pointed out by Kessler et al. [19], for the interpretation of the experiments it is more appropriate to use a quenched noise in (2.19), $\eta(x, h)$, and this is the version we shall discuss below.

At the places where the surface is locally almost pinned (slowed down) $\partial h/\partial t \ll 1$. On the other hand, at the same locations $\nabla^2 h + \lambda/2(\nabla h)^2 \gg 1$. According to (2.19) this can hold only if $-(v + \eta) \gg 1$ in these points. We argue that large negative values of the noise η are not physical, because this would mean that a flat surface in the given point would move with a large velocity in the direction *opposite* to the growth. Since the fluid is wetting, its spontaneous motion cannot be reverse.

Nevertheless, the equation (2.19) with quenched noise can be solved numerically making various assumptions for η. Kessler et al. [19] solved the KPZ equation in the absence of the nonlinear term (so for $\lambda = 0$) using quenched noise. Without mentioning the details, we would like to point out that such an approach does not lead to surfaces similar to the experimental ones.

Since our main goal is to understand what are the most relevant factors determining the behaviour of experimental surfaces, we have numerically

Figure 3.1: Subsequent interfaces obtained by numerically integrating equation (3.1) for $p = 0.0001$ and $v = 0.5$ for a system of linear size $L = 1500$. Here each interface corresponds to a fixed t.(a) $\lambda = 1$, (b) $\lambda = 0$

studied (3.1) for times and system sizes compatible to those which have been realized in the wetting experiments of Rubio et al. [15] and of Horváth et al. [16]. It is straightforward to integrate (3.1) numerically, the associated questions we discussed earlier in subsection 2.2.5 describing the numerical solution for both the quenched and time dependent noise cases. We have assumed that $p+\eta$ is always larger than zero, thus, the surface never becomes completely pinned. On the other hand, at places where $p+\eta \ll 1$, the motion of the interface slows down dramatically. These points can be considered as temporarily pinned. Like in all of the existing experiments on growth involving flow of matter, after some time the surface passes by these places or regions of low permeability and advances further without a complete stop.

For simplicity we assumed that η was distributed uniformly on (0,1]. We calculated the surfaces for the following set of parameters: system sizes $L = 800$ and $L = 1500$ with $p = 0.0001$ and $v = 0.5$ for $\lambda = 1$ and $\lambda = 0$. Figure 3.1 displays the numerical interfaces for $L = 1500$.

It should be pointed out that in the present case the mesh size used in

Figure 3.2: (a) The time dependence of the surface width w for various values (ranging from 0.0001 to 1) of the parameter p related to the strength of the pinning forces (smaller p corresponds to stronger pinning). There is a well defined crossover at a time t_c, depending on p, from a scaling according to an exponent $\beta \simeq 0.65$ to a scaling with β about 0.26. These results were obtained for by averaging over 20 runs of 50000 time steps for system sizes $L = 1500$. (b) The behaviour of the crossover time t_c as a function of the parameter p. In a limited region the dependence can be approximated as $t_c \sim p^{-0.7}$.

the course of discretizing the x dependence in (3.1) has a physical meaning: it corresponds to the lover cutoff length scale of the fluctuations of the media (for example, it can be identified with the diameter of the glass beads in the series of experiments mentioned above, since η is assigned to the grid points of a square lattice with mesh size Δx). In t a finer discretization is used, and the actual value of h is a quasi continuous variable.

The simulated surfaces look very similar to the observed ones. Interestingly, the EW case ($\lambda = 0$) resulted in interfaces having a closer resemblance to the experimental ones, although there is no particular reason to think that lateral growth can be neglected during the development of wetting fronts.

Next we investigated $w(L, t)$, the time dependence of the width of the entire system. The results shown in Figure 3.2a indicate that at early times there exists a non-trivial scaling

$$w \sim t^{\beta} \tag{3.5}$$

Figure 3.3: The distribution of the noise values (output noise) along the surface for $t \gg t_c$. The solid line is for $p = 0.0001$, the thin line is for $p = 0.0003$, the dotted line is for $p = 0.001$.

with $\beta \simeq 0.65 \pm 0.05$ in a surprisingly good agreement with the only published experimental result [16]. The crossover to a behaviour described by a smaller exponent $\beta = 0.26 \pm 0.05$ is well pronounced and according to our simulations the crossover time t_c only weakly depends on L. Our preliminary calculations indicate that for larger system sizes and longer times the value 0.26 does not change significantly. The crossover time has a dependence on p which in a limited region of the p values can be interpreted in terms of power law scaling. This is demonstrated in Figure 3.2b. Assuming that for the intermediate values $t_c \sim p^{-\gamma}$, a linear fit to the data gives the estimate $\gamma = 0.7 \pm 0.1$.

We have also calculated the spatial scaling of w. According to our results for $L = 800$ and 1500 there exist no well defined, extended straight parts in the $\log w$ versus $\log r$ plots for the sizes and times we could realize. However, for larger sizes ($L = 5000$) a scaling of $w(r)$ as a function of r over a limited range of length scale could be observed (just as in the EW case of the quenched additive noise). The corresponding exponent $\alpha \simeq 0.47$ was close to 0.5.

The actual status of the growing surface can be characterized by the distribution $P(\eta)$ of η values. We consider a large set of surfaces obtained for times $t \gg t_c$ and determine the number of lattice sites with a given η. The time the interface spends in a particular grid point (with the corresponding

Figure 3.4: Series of surfaces obtained as a function of time for the model with η depending on x only (see the text).

η) strongly depends on the value of η as well as on the local derivatives of the surface. These factors lead to a $P(\eta)$ which is rather different from the original uniform distribution for η. The results are presented in Figure 3.3. This figure suggests that in the limit of very small p there is a range of η in which the distribution of the random numbers along the interface scales with an exponent close to 0.5. Again, a trivial, Gaussian type input noise distribution is transformed by the growth mechanism into a power law distribution of the noise values along the interface.

An interesting special case of the noise is when η depends only on x. An existing aspect of the physics is reflected by this choice: the motion of the interface is determined by not only the conditions at the surface, but also by the permeability of regions already left behind (which may partially block the supply of additional fluid). A possible realization of this case includes a Hele-Shaw cell with parallel grooves of different depth engraved onto one of the glass plates.

Figure 3.4 shows a typical series of surfaces for $L = 1500$, $p = 0.0001$ and $v = 0.5$. In this model there is a well pronounced scaling both in time

and space, with numerically determined exponents close to 1 ($\alpha \simeq \beta \simeq 0.96 \pm 0.06$). A temporal scaling with an exponent 1 can be considered as a trivial consequence of the particular choice for the noise. On the other hand, the result $\alpha = 1$ is far less trivial and indicates that the surfaces attain a limiting case when the interface is both a single valued self-similar (and self-affine) function.

In conclusion, we have proposed an approach which is intended to take into account the experimental conditions during two-phase fluid flows in inhomogeneous media as well as possible. By introducing a stochastic partial differential equation with a multiplicative noise describing the development of the interface we have been able to obtain (i) surfaces remarkably similar to those observed in the experiments (ii) a scaling behaviour of the surface width with an exponent being in an excellent agreement with the measured value. (iii) In addition, the transformation of the uniform input noise to a power law distribution of the η values along the surface could be observed.

3.2 Results related to the deterministic growth equation

3.2.1 Numerical results

Here we present our simulation results of ([29],[30]) concerning the singular interface equations (2.21) of Zhang. We show by numerical integration that the discretized (and parametrized) version of these simple deterministic partial differential equations exhibit rich spatiotemporal behaviour representing a *mixture of stochastic and deterministic regimes.*

We study the following variants of (2.21)

$$\frac{\partial h}{\partial t} = \nabla^2 h - B \ln(|\nabla h| + A) \tag{3.6}$$

and

$$\frac{\partial h}{\partial t} = \nabla^2 h + B|\nabla h + A|^{\alpha}. \tag{3.7}$$

The parameters $A > 0$ and B are used to control the weight of the singular term.

Our main goal is to demonstrate the various interesting phenomena which are exhibited by equations (3.6), (3.7) *as B is increased from 0.* We shall use the following approach: (i) start with random or some simple initial surface (no relevant difference has been seen between the two kinds of simulational results), (ii) numerically integrate the equation using a simple discretization scheme (iii) evaluate the data in terms of the surface roughness (the total width) $w(t)$ of the advancing surface given by the function $h(t)$ and the height-height correlation function $c(x)$ (for some t). In the computations of the surface width by (2.11) and of $c(x)$ by $c(x) = \langle |h(x + \Delta x) - h(x)| \rangle_x$ the averaging is made over the $h(x)$ values for $x = 1, ..., L$ at time t. All our simulations are carried out in a $1 + 1$ dimensional strip with periodic boundary conditions.

At first we shall pay most of our attention to the numerical solution of equation (3.6). We use the discretization scheme similar to (2.24)

$$\begin{aligned} h(x, t + \Delta t) &= h(x, t) + \Delta t \ \ (h(x - 1, t) - 2h(x, t) + h(x + 1, t)) - \\ &\quad -B \ \Delta t \ \ (\ln(|(h(x + 1, t) - h(x - 1, t)| + A)) \,. \end{aligned} \tag{3.8}$$

Since we are considering periodic boundary conditions the solutions must have extrema (or at least one extremum point). In the case of continuous

Figure 3.5: Subsequent snapshots of the evolving surface obtained by numerically integrating eq. (3.6) for $L = 512$, $A = 0.0002$ and $B = 0.002$ (a); $B = 0.0053$ (b); $B = 0.0061$ (c) and $B = 0.01$ (d). All surfaces have been shifted by an amount $-C(B)t$ (this is equivalent to including an extra, irrelevant term $-C$ into the RHS of Eq. (3.6)) in order to show many surfaces (othervise separated by a much larger gap) in the available area of a figure. In addition, the solutions are stretched in the vertical direction (multiplied by a factor, depending on B, in the range of 200 - 2000 to enhance the details.)

solutions at an extremum point either the term $\ln(|\nabla h|)$ (smooth extremum) or the term $\nabla^2 h$ (sharp kink) diverges. Discretization eliminates this sort of divergences because starting with random initial conditions the finite difference expression for the gradient takes on the value $\nabla h = 0$ with zero probability while for $\nabla^2 h$ it is always finite even at the sharpest extrema.

For the integration step Δt in time we used in most of the cases 0.05 (the results did not depend on Δt for $\Delta t < 0.1$). The width of the strip was typically $L = 512$ grid points, but we have also carried out simulations for $L = 256$ and $L = 1024$ to check whether there is any significant size-dependence in our calculations. The parameter A was kept constant and B, the relative weight of the singular term, was increased gradually from zero. The initial condition $h(x, 0)$ was a random surface with heights uniformly distributed between 0.0 and 0.01. We fulfilled the computations with some simple initial functions also, e.g., $p \sin(4\pi x/L) + q$ ($p > 0$ parameter, $q > 0$ is a small constant).

Our findings are demonstrated in Figures 3.5–3.8. First we present (Fig. 3.5a–d) sets of actual surface configurations for various B to illustrate the qualitative behaviour of the solutions.

(i) Naturally, for $B = 0$ the surface becomes perfectly *smooth* as $t \to \infty$ since, as can be seen from a trivial linear stability analysis, the surface tension-like term $\nabla^2 h$ leads to the dying out of the perturbations.

(ii) As B becomes larger, at places where ∇h is approximately zero the term $B \ln(|\nabla h| + A)$ is close to $B \ln(A)$ which, for $A \ll 1$, represents a large perturbation to the local velocity of the advancing surface. The strength of this perturbation sensitively depends on how close is ∇h to zero at the given discretization node and this feature, through the nonlinearity of the dependence of the velocity on the local slope, results in the *roughening* of the surface (Fig. 3.5a).

(iii) For $B > B_L$ the surface becomes piecewise *linear*, consisting of straight line segments of a given slope (Fig. 3.5d). It is natural that the singular term dominated regime is made of straight line segments which (a) minimize the number of points where $\nabla h = 0$ and, (b) correspond to a trivial steady state because for these segments $\nabla^2 h = 0$ and $\nabla h = \text{const}$.

(iv) Perhaps most interestingly, the crossover from stochastic to piecewise behaviour is accompanied with a phenomenon analogous to *intermittency*: periods of almost perfectly regular (piecewise) growth regimes are interrupted with intervals of stochastic growth (Fig. 3.5c). As an intermediate regime we can also observe surface evolution during which parts of the surface become

Figure 3.6: The total width of the growing surfaces $w(t)$ as a function of time for $A = 0.002$ and $B = 0.0061$. The intermittent nature of the solution is demonstrated by the periods of steady state regime (relatively large, constant value of w corresponding to a piecewise linear solution existing for some time) interrupted by stochastically fluctuating time dependence.

piecewise linear and turn random at later stages while the rest of the surface remains disordered (Fig. 3.5b).

In order to describe the above changes in the spatio-temporal behaviour in a more quantitative manner we calculate the total width of the surfaces. The *intermittent* nature of the solution of Eq. (3.6) for $B = 0.0061$ is demonstrated in Fig. 3.6. Intervals of the steady state regime (relatively large, constant value of w corresponding to a piecewise linear solution existing for some time) are interrupted by stochastically changing behaviour.

Fig. 3.7a shows how $W = w(t \to \infty)$ depends on the *relative weight B of the nonlinear term* for $A = 0.0001$. In this plot the $\log(W)$ values approximately follow two straight lines as a function of $\log(B)$ indicating a power law dependence of the total surface width in a certain range of the parameter B. For small B the slope is about 3, while for larger B the slope is close to 1. As discussed above the discretized version of the term $\ln(|\nabla h|)$ never becomes equal to infinity; in the simulations the role of A is to introduce a largest possible value of the nonlinear term. Thus, the size of the scaling region and the value of B at which the crossover takes place depend on the value of A. Fig. 3.7b shows the results for $A = 0$. In this case the data fall onto a straight line over many decades because the term $\ln(|\nabla h|)$ can assume much larger (but still finite) values than $\ln(|\nabla h + A|)$ for $A > 0$.

We have investigated also the geometry of the surface by calculating the

Figure 3.7: The dependence of the steady state width W on the weight of the singular term B for Eq. (3.6). (a) $A = 0.00001$ (b) $A = 0$. The approximately straight part indicates scaling over a limited region of the B values. The slope of the straight lines in (a) are approximately 1 and 3, while in Fig. 3.7b the slope is equal to 1. Here the data scale according to an exponent (slope of the line) approximately equal to 0.68. These results were obtained by averaging over 100 runs and 200 surfaces/run.

Figure 3.8: The height-height correlation function $c(x)$ for $A = 0.0002$ and $B = 0.002$. The self-affine fractal nature of the growing surface is indicated by the straight part in the plot. The slope corresponds to a roughness exponent $H \approx 0.7$.

Figure 3.9: The dependence of the steady state width W on the weight of the singular term B for Eq. (3.6). with $\alpha = -1/2$.

height-height correlation function (for some t) $c(x)$. The fractal roughness of the growing surface for $B = 0.002$ is indicated by the straight part in the plot of $\log c(x)$ as a function of x (Fig. 3.8). The corresponding roughness exponent is $H \approx 0.7$, where H is defined by the expression $c(x) \sim x^H$.

In conclusion, we have shown that the discretized version of simple deterministic partial differential equations with singular terms (Zhang equations) exhibit a behaviour which is an interesting *mixture of stochastic and deterministic regimes*. Varying the relative strength B of the singular term we have been able to detect transitions in the global behaviour of the solutions in analogy with some viscous flows in which changes from laminar to intermittent and turbulent regimes take place as the Reynolds number is increased. In our case the emergence of the new type of solution depends on B as a power law with a well defined exponent. The piecewise linear solution we find numerically may be related to the 'groove' instability observed in several surface growth models.

In the following we consider the parametrized Zhang equation (3.7). with the power term. By increasing B we can make the relative role of the nonlinearity stronger, while increasing A "softens" the nature of the singularity (the relative change of the singular term for small gradients is decreased).

In [29] we investigated (3.7) for $\alpha < 0$. Fig. 3.9 displays the total width versus B for $\alpha = -1/2$. It demonstrates that the behaviour of W is essentially the same as it was for equation (3.6) independently of the actual form of the singular term. The slope corresponding to the surprisingly straight set of data is ≈ 0.68. The extension of this behaviour depends on the actual value

of A. The value of the parameter A has a simple effect of a cutoff of scaling for smaller B. As $A \to 0$ the almost perfect scaling behaviour extends over many orders of magnitude.

Then in [30] we study the case $\alpha > 0$ in (3.7) which is quite different since the singular term for such an exponent does not diverge as the gradient goes to zero.

We integrate equation (3.7) using the finite difference scheme (2.24) while discretizing the singular part in (3.7) by

$$B\ \Delta t\ (|\ (h(x+1,t) - h(x-1,t)| + A)^{\alpha}.$$

Most of the parameters of the scheme are the same as previously. We take for the integration step Δt in most of the cases 0.05 (the results did not depend on Δt for $\Delta t < 0.1$). We used $\alpha = 1/2$ for the exponent and the width of the strip was typically $L = 512$ grid points. We have also carried out simulations for $L = 256$ and $L = 1024$ to check whether there is any significant size-dependence in our calculations. The parameter A was kept constant and B, the relative weight of the singular term, was increased gradually from zero. The initial condition $h(x,0)$ was a random surface with heights uniformly distributed between 0.0 and 0.01.

The qualitative aspects of our findings are illustrated in Figure 3.10, where two sets of actual surface configurations for two selected B values and for $A = 0.01$ are shown (for $B = 0$ the surface becomes perfectly smooth as $t \to \infty$ since, as can be seen from a trivial linear stability analysis, the surface tension-like term $\nabla^2 h$ leads to the dying out of the perturbations).

For $B = 5$ the interplay of the instability mentioned above and the smoothening effect of the Laplacian term results in a rough surface. (Fig. 3.10a). As B is decreased ($B = 1$) the surface develops parts which are close to linear and travel along the x axis. These wave-like parts may collide and annihilate as is demonstrated by Fig. 3.10b. The total width of the surface is rather small in this case which is compensated by streching the curves in the vertical direction by a factor 100. Subsequent "snapshots" of the evolving surface obtained by numerically integrating eq. (3.7) for $L = 512$, $A = 0.01$ and (a) $B = 5$ and (b) $B = 1$. All surfaces have been shifted by an amount $-C(B)t$ (this is equivalent to including an extra, irrelevant term $-C$ into the RHS of Eq. (3)) in order to show many surfaces (othervise separated by a much larger gap) in the available area of a figure. In addition, the solutions in (b) are "stretched" in the vertical direction by a factor 100.

Figure 3.10: Subsequent snapshots of the evolving surface obtained by numerically integrating eq. (3.7) for $L = 512$, $A = 0.01$ and (a) $B = 5$ and (b) $B = 1$. All surfaces have been shifted by an amount $-C(B)t$ (this is equivalent to including an extra, irrelevant term $-C$ into the RHS of Eq. (3.7)) in order to show many surfaces (othervise separated by a much larger gap) in the available area of a figure. In addition, the solutions in (b) are stretched in the vertical direction by a factor 100.

Fig. 3.11 shows how $W = w(t \gg 1)$ (for $t = 25000$) depends on the *relative weight B of the nonlinear term* for two values of A. In this plot $\log(W)$ approximately follows two straight lines as a function of $\log(B)$ indicating a power law like dependence of the total surface width beyond some A dependent threshold value of B. For small B the plots converge to a constant, while for larger B the slope of the line fitted to the data on this log-log plot corresponds to an exponent approximately equal to $\delta = 0.5$. Thus, B plays the role of a control parameter and the change in the behaviour can be interpreted in terms of a morphological phase transition of the rough surface (see [4]). The value of the parameter A has a simple effect of a cutoff of scaling for smaller B. As $A \to 0$ the almost perfect scaling behaviour extends over many orders of magnitude. For $t \to \infty$ and $B = 0$ the surface width should go to zero; however, this convergence is very slow. Thus, in the limit $t \to \infty$ for $A = 0$ the scaling may extend down to $B = 0$.

A very peculiar effect can also be observed in Fig. 3.11. For $A > 0$ the surface width shows a sharp minimum at an A dependent position. There is only one reasonable explanation for this phenomenon: for some B the singular term leads to the *smoothening (!)* of the surface. For $B = 0$ and $t \to \infty$ the surface should be perfectly smooth. The convergence to this limit

Figure 3.11: The dependence of the width $W = w(t = 25000)$ on the weight of the singular term B for Eq. (3.7). (o) $A = 0$; (Δ) $A = 0.01$. The approximately straight part indicates scaling over a limited region of the B values. The slope of the straight part is approximately 0.5.

is, however, very slow. Apparently, the *rate* of convergency to the smooth solution is drastically increased by the nonlinearity in a given region of B values.

We have investigated also the geometry of the surface by calculating the height-height correlation function $c(x)$ (for some t). The fractal roughness of the growing surface for $B = 5$ and $A = 0.01$ is indicated by the straight part in the plot of $\log c(x)$ as a function of x (Fig. 3.12). The corresponding roughness exponent is $H \approx 0.7$, where H is defined by the expression $c(x) \sim x^H$. In the regime where the surface has mainly linear parts H is approximately equal to 1.

Remark. The simulation and the surface drawing programs have been written in Pascal, and later on some of them had C versions. During the years the numerical simulations have been carried out in workstations (SUN OS 4.1.3, Solaris 2.3 etc) and main frames (like IBM RISC 6000) provided at different places: at the Computer and Automation Center H.A.S. (SZTAKI), at the Supercomputing Centre (HLRZ), KFA Jülich and at the Budapest University of Economics. The calculations have been very CPU time consuming. For a given parameter set A, B we considered as one numerical experiment

Figure 3.12: The height-height correlation function $c(x)$ for $A = 0.01$ and $B = 5$. The self-affine fractal nature of the growing surface is indicated by the straight part in the plot. The slope corresponds to a roughness exponent $H \approx 0.7$.

the computations of our quantitative measures $w(t)$ and $c(x)$ with one initial function. Then for several hundred times we repeated the numerical experiment for the same A,B but different initial functions (in case of the random initial conditions, naturally, each run becomes different) and took the average of $w(t)$ and $c(x)$ by the number of experiments.

3.2.2 Analytic results: special solutions

In [31] we obtained analytical results for the singular interface equation of Zhang

$$\frac{\partial u(x,t)}{\partial t} = \nabla^2 u(x,t) + \ln(|\nabla u|) \tag{3.9}$$

and a closely related more general equation

$$\frac{\partial u(x,t)}{\partial t} = \nabla^2 u(x,t) + \delta u_x^2 + \ln(|\nabla u|). \tag{3.10}$$

(For the sake of mathematical traditions we used here $u(x,t)$ instead of $h(x,t)$.)

In the previous section the finite difference version of a slightly modified form of the singular interface equation (3.9) has been numerically investigated for the Cauchy-Dirichlet problem with periodic boundary condition where the initial function was a non-negative noise function with $u_x(x,0) = 0$ at several points [29]. Our numerical calculations (beside other results) have shown that after some time (for large t) the typical form of the solution is like the one in Figure 3.13. Here the minimum points correspond to those values of x (for fixed t) where $u_x = 0$. In the neighbourhood of the two local minima the solution looks like a linear function which seems to be logical because x and $-x$ are solutions to equation (3.9). On the other hand, the function $|x|$ is not a classical solution due to a lack of smoothness at zero (the flux is not continuous). It is easy to see that $|x|$ is not a weak solution either (see the definition of weak solution below). The analytical approach could provide us with a possible explanation how the typical forms like in Figure 3.13 can arise.

Our results show the existence of special solutions namely travelling waves (TW) and self-similar solutions which have linear asymptotics, at singular points have continuous first derivatives consequently they are solutions in the weak sense.

We shall see that $u(x,t)$ has no continuous second derivative with respect to x at the points where $u_x = 0$. In the neighbourhood of such points we indicate in what sense the solutions $u(x,t)$ satisfy equations (3.9) and (3.10). This is the usual definition of weak solutions in the theory of partial differential equations (see, e.g., [21]). The identity (3.11) is the result of multiplication of (3.10) by $\varphi(x,t)$ and of formal integration by parts.

Figure 3.13: Typical form of the numerical solution to equation (3.9) for fixed (large) t. The minimum points correspond to those values of x (for fixed t) where $u_x = 0$.

Weak solution. We shall say that $u(x,t)$ is a weak solution to equation (3.10) if the integral identity

$$\int_{x_0}^{x_1} u\varphi|_{t_0}^{t_1} dx = \int_{x_0}^{x_1}\int_{t_0}^{t_1} (u\varphi_t - u_x\varphi_x + \delta u_x^2\varphi + \varphi \ln|u_x|)dxdt \tag{3.11}$$

is satisfied for all rectangles $R = [x_0, x_1] \times [t_0, t_1] \in (-\infty, \infty) \times (0, \infty)$ and smooth (on R) functions $\varphi(x,t)$ such that $\varphi(x_0,t) = \varphi(x_1,t) = 0$.

Note that this definition requires only the integrability of functions u, u_x, u_x^2, $\ln|u_x|$ and does not contain u_{xx}.

Travelling wave. The travelling wave (TW) solution to equations (3.9) and (3.10) is a solution of the form $u = g(\xi)$, where $\xi = x - \lambda t$ and λ is a real number (speed) [26].

If function $g(\xi)$ is to be a function providing a TW solution then it should satisfy the following second order ordinary differential equation

$$g'' + \lambda g' + \delta g'^2 + \ln|g'| = 0.$$

Using the substitution $g' = f$ we get

$$f' + \lambda f + \delta f^2 + \ln|f| = 0. \tag{3.12}$$

First we consider the case $\delta = 0$ (equation (3.9)) which turned out to be

more general from our point of view. Then equation (3.12) reads

$$f' = -\lambda f + \ln \frac{1}{|f|}. \tag{3.13}$$

Here we shall study equation (3.13) with $\lambda > 0$ in detail; the $\lambda < 0$ case can be handled analogously.

The roots of the non-linear equation

$$-\lambda f + \ln \frac{1}{|f|} = 0 \tag{3.14}$$

determine the equilibrium points (where $f' = 0$) of (3.13) .

Remark 3. *If the constants f_i are equilibrium points of (3.13) then the linear functions $u = (x - \lambda t) f_i$ will be TW solutions to equation 3.9.*

In the following we shall consider the nontrivial TW solutions to (3.9).

Remark 4. *In each interval not containing any of the equilibrium points, the function*

$$F(f) := \int^f \frac{ds}{\ln \frac{1}{|s|} - \lambda s} = \xi \tag{3.15}$$

is strictly monotone (increasing or decreasing). So the inverse function, F^{-1}, exists in this interval and the solution to equation (3.13) is the function

$$f(\xi) = F^{-1}(\xi)$$

which gives us the solution to (3.9):

$$u = g(\xi) = \int f(\xi) d\xi + \mathrm{c}, \qquad c \text{ is a constant.}$$

Let $\lambda_0 = e^{-1}$, ($\ln\ e = 1$). Depending on the speed of the travelling wave λ, we shall have three different cases.

I. If $0 < \lambda < \lambda_0$ then equation (3.13) has three equilibrium points. Namely equation (3.14) has exactly three roots: f_0, f_1, f_2, where $0 < f_0 < 1$, $f_1 < -1$ and $f_2 < f_1$.

II. If $\lambda = \lambda_0$, then equation (3.14) has two roots: f_0, f_1, where $0 < f_0 < 1$, $f_1 = -e$.

III. If $\lambda > \lambda_0$ then we have only one equilibrium point $0 < f_0 < 1$.

Figure 3.14: Function $F'(f)$ used to construct $u(x-\lambda t)$, the TW solutions to equation (3.9) in case $0 < \lambda < \lambda_0$.

Case I: $0 < \lambda < \lambda_0$
Here equation (3.13) has four different solutions separated by equilibrium solutions f_i $(i = 0, 1, 2)$. The solution between f_1 and f_0, is the only one which becomes 0 in one point. Because $f = g' = u_x$, the original equation (3.9) is genuinely singular there.
In the following we construct TW solutions by the help of function $F(f)$ of (3.15) as described in Remark 4. The starting point our proofs is the function $F'(f)$ (see Figure 3.14).
(i) $-\infty < f < f_2$. In this interval $F' > 0$, $F' \to +\infty$ when $f \nearrow f_2$ and $F' \searrow 0$ when $f \to -\infty$. The function, F, is strictly monotone increasing,

$F \to +\infty$ if $f \nearrow f_2$ as $-\ln|f-f_2|$ and $F \to -\infty$ for $f \to -\infty$ as $-\ln(-f)$. Consequently, the function $f(\xi)$ for large $\xi > 0$ behaves like $-e^{-\xi} + f_2$, for large negative ξ like $-e^{-\xi}$. Integration gives the function $u = g_1(\xi)$ which has asymptote $f_2\xi$ if $\xi \to +\infty$ and is like $e^{-\xi}$ for large negative ξ.
(ii) $f_0 < f < +\infty$. Here $F' < 0$, F is strictly decreasing, $F \sim -\ln|f-f_0|$ if $f \searrow f_0$,and F behaves like $-\ln f$ for large f.
Hereafter $a(x) \sim b(x)$ means that $\lim_{x\to 0} \frac{a(x)}{b(x)} = \mathrm{c}$, where c is a positive constant.
The function $f(\xi)$ decreases from ∞ to f_0 and globally behaves like $e^{-\xi} + f_0$. The corresponding solution, $u = g_2(\xi)$, has $f_0\xi$ as its asymptote for large positive ξ and behaves like $-e^{-\xi}$ for large negative ξ. Thus, basically, g_2 looks like $-g_1(\xi)$.
(iii) $f_2 < f < f_1 < -1$. In that case, as it is easy to see, we have a bounded negative $f(\xi)$ such that $f(-\infty) = f_1$ and $f(+\infty) = f_2$. Thus, $u = g_3(\xi)$ is like a hyperbole with asymptotes $f_1\xi$ for large negative ξ and $f_2\xi$ for $\xi \to +\infty$. The TW solutions, $g_1(\xi)$, $g_2(\xi)$, $g_3(\xi)$ for which u_x never turns to zero, are presented in Figure 3.15.
(iv) $f_1 < f < f_0$. This is the first important case: the derivative of the corresponding solution becomes zero at some point (without a loss of generality, we can suppose that it happens at the origin $x = 0$).
In the interval (f_1, f_0) the function $F'(f)$ is nonnegative, $F'(0) = 0$ and $F''(\pm 0) = \pm\infty$. In the neighbourhood of f_0 and f_1 the function F' behaves like $|f-f_i|^{-1}$. The function F is strictly monotone increasing, $F \to -\infty$ if $f \to f_1$ and $F \to +\infty$ for $f \to f_0$. Consequently, the function $u = g_4(\xi)$ decreases to zero and is increasing from zero. It is a non-negative hyperbole-like function with asymptotes $f_1\xi - \xi_0$ from the left and $f_0\xi - \xi_1$ from right, $\xi_i > 0$, see Figure 3.16.
The function $F'(f)$ for small f behaves like $(\ln\frac{1}{|f|})^{-1}$, thus $F(f) \sim f(\ln\frac{1}{|f|})^{-1}$. It is easy to see that $f(\xi) \sim |\xi| \ln\frac{1}{|\xi|}$ for small $|\xi|$, so

$$g_4(\xi) \sim \xi^2 \ln\frac{1}{|\xi|}, \qquad \text{for small } \xi.$$

One can see that the second derivative of $g_4(\xi)$ at zero is not continuous: $g_4''(\xi) \sim \ln\frac{1}{|\xi|} \to +\infty$ when $|\xi| \to 0$. In contrast to (3.9) identity (3.11) does not contain u_{xx} and all the integrals in (3.11) exist except, possibly, the last one $\int \varphi \ln|u_x| dx$. If $\varphi = 1$ in the ε -neighbourhood of zero (we suppose that $u_x = 0$ at zero) then the convergence of this integral is equivalent to the

Figure 3.15: Travelling wave solutions ($u = g_1(\xi), u = g_2(\xi), u = g_3(\xi)$, where $\xi = x - \lambda t$) of equation (3.9) for the case when u_x never turns to zero.

Figure 3.16: Travelling wave solution of equation (3.9) when $u_x = 0$ at some point (without loss of generality we suppose that at $x = 0$, for fixed t). It has the cusp-like form similar to Figure 3.13.

convergence of $\int_{-\varepsilon}^{\varepsilon} \ln(|x| \ln \frac{1}{|x|})dx$. However,

$$|\ln(|x| \ \ln \frac{1}{|x|})| \leq |\ln|x|| + |\ln \ln \frac{1}{|x|}| \leq c \ |\ln|x||$$

which is integrable at zero.
Case II: $\lambda = \lambda_0$. Equation (3.14) has two zeros : $f_0 \in (0,1)$ and $f_1 = -e$. The function $F'(f)$ is the same as in Figure 3.14 with $f_2 = f_1$. Thus, we have three travelling waves which behave qualitatively like g_1, g_2 and g_4 from the previous case.
Case III: $\lambda > \lambda_0$. The travelling wave corresponding to $f > f_0$ is like g_2. Let us now assume that $f < f_0$. The function $F'(f)$ in the interval $[-\varepsilon, f_0)$, $\varepsilon > 0$ behaves like $F'(f)$ in Figure 3.14, but decreases to zero when $f \to -\infty$ like $-\frac{1}{f}$ having a maximum at some point $f_3 < -\varepsilon$. The corresponding solution, $u = g_5(\xi)$, behaves like g_4 in the neighbourhood of zero, while for large positive ξ it has a linear asymptote $f_0\xi - \xi_0$ and for large negative ξ behaves like $e^{-\xi}$. In the case $\lambda = 0$ (stationary TW) we have $F'(f) = -\frac{1}{\ln|f|}$.

Here there are two equilibria $f_0 = 1$, $f_1 = -1$. The travelling wave between $f_1 < f < f_0$ is qualitatively the same as g_4 while for $f_0 < f$ the solution is like g_2.
When $f < -1$ the TW solution $u = g_6(\xi)$ is a strictly monotone decreasing function having ξ as an asymptote for large negative ξ and behaves like $\xi^2 \ln \frac{1}{\xi}$ for large positive ξ.

The case $\delta > 0$ (equation (3.10)), $\lambda > 0$ is qualitatively the same as the previous one ($\delta = \lambda = 0$): one has two equilibria ,f_3 and f_4, such that $f_4 < 0 < f_3 < 1$.

Now we deal with a self-similar type solution to equation (3.9) and describe its geometrical properties. This solution will have the form

$$u(x,t) = (t+t_0)^{\alpha} g(\frac{x}{(t+t_0)^{\beta}}) + f(t) \tag{3.16}$$

where the functions $g(\xi)$, $f(t)$ and the positive constants α, β are to be determined.
Formula (3.16) expresses the *self-similar* nature of the solution, or can be regarded as *solution with dynamic scaling.* Here we refer to dynamic scaling because equation (3.16) has a form which is analogous to the scaling behaviour of self-affine growing surfaces (see, e.g., in [5] equation 7.19) whose properties can be described in terms of dynamic scaling.

Theorem 1. *Let $g(\xi)$ be the solution of the generalized Weber equation*

$$g(\xi) - \frac{1}{2}\,\xi\; g'(\xi) = g''(\xi) + \ln|g'(\xi)|. \tag{3.17}$$

Then
1) the function

$$u(x,t) = (t+t_0)[g(\xi) + \frac{1}{2}(\ln(t+t_0) - 1)], \quad \xi = \frac{x}{\sqrt{(t+t_0)}}$$

satisfies equation

$$u_t = u_{xx} + \ln|u_x|.$$

2) Function $g(\xi)$ has the following geometrical properties

(i) $g(\xi)$ is monotonously increasing for $\xi > 0$ and $g(\xi)$ is monotonously decreasing for $\xi < 0$,

(ii) $g(\xi) \sim \xi^2 \ln\frac{1}{|\xi|}$, for small $|\xi|$,

(iii) $g(\xi) \sim \xi^2$, for large $|\xi|$.

Remark 5. *We see that $g(\xi)$ roughly looks like ξ^2 (we suppose, as before, that $g(0) = 0$.) The only important difference is the nonsmoothness of g at zero: the second derivative blows up at $\xi = 0$. The next to leading order term in (ii) is $\xi^3 \ln\frac{1}{|\xi|}$.*

Remark 6. *It follows from (3.17) that if $g\xi)$ is a solution then $h(\xi) = g(-\xi)$ also satisfies (3.17). Since $g \equiv$ constant is not a solution, it is possible to show, that for $\xi > 0$ the initial value problem for (3.17) with $g(0) = 0$, $g'(0) = 0$ has a unique global solution $g = g^+(\xi)$. For $\xi < 0$ we set $g = g^+(-\xi)$. At the point $\xi = 0$ the function $g(\xi)$ is not necessarily smooth ($g''(0)$ can blow up) but we can understand equality (3.17) in the neighbourhood of $\xi = 0$ in a weak sense, as in definition of the weak solution for 3.9.*

Proof of 1) Substitution to 3.9 gives

$$\begin{aligned} \alpha(t+t_0)^{\alpha-1} g(\xi) - \beta(t+t_0)^{\alpha-1}\,\xi\; g'(\xi) + f'(t) &= \\ (t+t_0)^{\alpha-2\beta} g'' + \ln|(t+t_0)^{\alpha-\beta} g'(\xi)| &= \\ (t+t_0)^{\alpha-2\beta} g'' + (\alpha-\beta)\ln|(t+t_0)| + \ln|g'(\xi)|. & \end{aligned}$$

Now, one can see that if we take

$$f(t) = \frac{1}{2}(t+t_0)\,[\ln(t+t_0) - 1], \quad t_0 \geq e, \quad \alpha = 1 \quad \text{and} \quad \beta = \frac{1}{2},$$

$u(x,t)$ will be a solution to 3.9 provided that $g(\xi)$ satisfies equation (3.17).
Proof of 2)
(i) It is sufficient to show that $g'(\xi) > 0$ for $\xi > 0$.
In fact, suppose that ξ_1 is the first value where $g'(\xi)$ is zero. Let us take $\xi_2 = \xi_1 - \varepsilon > 0$, where ε is a small positive number. One has $g''(\xi_2) < 0$ and $\ln|g'(\xi)|$ is a large negative number. However, in the same neighbourhood the left hand side of (3.17) is positive. So $g'(\xi) > 0$ for $\xi > 0$.
(ii) We can see from (3.17) that the behaviour of $g(\xi)$ in the right neigbourhood of $\xi = 0$ ($\xi > 0$) is controlled by equation

$$g_1''(\xi) + \ln|g_1'(\xi)| = 0.$$

By setting $g_1'(\xi) = y(\xi)$, one has

$$y'(\xi) + \ln|y(\xi)| = 0$$

from which we have $y(\xi) \sim \xi \ln\,\frac{1}{\xi}$, for $\xi \in (0,\varepsilon)$, $\quad \varepsilon > 0 \qquad$ is small, so

$$g_1(\xi) \sim g(\xi) \sim \xi^2 \ln\,\frac{1}{\xi}, \quad \text{for} \quad \xi \in (0,\varepsilon).$$

Thus, $g(\xi)$ at $\xi = 0$ (where $g' = 0$) behaves like $\xi^2 \ln\,\frac{1}{|\xi|}$, which means that $u(x,t)$ is like $x^2 \ln\frac{1}{|x|}$ for fixed t at $x = 0$ (where $u_x = 0$). This proves (ii).
(iii) First we show that $g(\xi)$ is at least power-like at infinity. Suppose the contrary:

$$\frac{g(\xi)}{\xi^{\varepsilon}} \to 0, \quad \textit{for} \quad \text{all} \quad \varepsilon > 0 \tag{3.18}$$

i.e. that $g(\xi)$ grows slower than any power of ξ. In that case, because of the monotonicity of g, we have $g'(\xi) \to 0$ as $\xi \to \infty$. Indeed, if $g'(\xi) \geq c > 0$ for $\xi > \xi_0$ then integration gives $g \geq c\,\xi$ which contradicts to (3.18). But if $g'(\xi) \to 0$, then the right-hand side of (3.17) goes to minus infinity. The only term of (3.17) which is able to balance it, is $-\frac{1}{2}\,\xi\,g'$, consequently $g'(\xi) \sim \frac{2}{\xi}\ln\xi$ for large ξ and $g \sim (\ln\xi)^2$. Substituting this into (3.17) and taking ξ large enough we obtain a contradiction.

Substitution $g(\xi) = \xi^\alpha$ into equation (3.17) gives

$$\xi^\alpha - \frac{\alpha}{2}\xi^\alpha = \alpha(\alpha-1)\xi^{\alpha-2} + \ln|\alpha\xi^{\alpha-1}|$$

which is true in the limit $\xi \to \infty$ only if $\alpha = 2$. For a more exact result, suppose that g has the form $g = \xi^2 h(\xi)$ where $\lim_{\xi\to\infty} \frac{h(\xi)}{\xi^\varepsilon} = 0$ for all $\varepsilon > 0$. Substitution into (3.17) leads to the equation

$$-\frac{1}{2}\xi h' = h'' + \frac{2\ h}{\xi^2} + \frac{4\ h'}{\xi} + \frac{1}{\xi^2}\ln|2\ \xi\ h + \xi^2\ h'|$$

from which we can see that the behaviour of $h(\xi)$ at infinity controlled by the equation

$$-\frac{1}{2}\xi\ h' = h''$$

having the explicit solution $h(\xi) = \int_0^\xi \varepsilon^{-\tau^2/4} d\tau$ with $h(+\infty) = \text{constant}$.

Chapter 4

Summary — Összefoglalás (in Hungarian)

Önaffin fraktál felületek dinamikája

Tevékenységünk elsősorban az önaffin fraktálfelületek dinamikájának aktuális kérdéseire irányult, melyeket a fizika vetett fel az 1980-as évek végétől kezdve. Azóta a terület óriási ütemű fejlődésnek indult, fontos eredmények születtek számítógépes szimuláció segítségével, valamint elméleti és kísérleti módszerekkel.

Az egyensúlytól távoli jelenségek osztályába tartozó önaffin növekedés számos dinamikus folyamat során fellép, amikor a növekvő határfelület új részek keletkezésével halad előre. Például a kristálynövekedés, permetezés, galvanizálás vagy biológiai növekedés folyamán. Fraktál felületek alakulhatnak ki anyagrétegek eltávolítása esetén is, így kémiai oldáskor, csiszolásnál, korrozió és erózió közben. A felületnövekedés más folyamatokkal is rokon jelenség, beleértve például a lángfrontok terjedését, a véletlen időpontokban megkevert folyadék hosszú idő elteltével kialakuló viselkedését, a szennyezések bekerülése miatt durvuló és lemaradó határfelületeket. A látszólag különböző, de egymással rokon jelenségek közötti összefüggések lehetővé teszik, hogy a durva felületek kialakulását többféle módon közelítsük meg [5].

Ha a növekedési folyamat feltételei olyanok, hogy a határfelület kialakulása marginálisan stabil (a fluktuációk hosszú ideig fennmaradnak nagyobb változás nélkül) és a fluktuációk lényegesek, a kialakuló struktúra durva felület lesz. Ez a felület jól leírható *fraktálfüggvények* - sehol nem differenciálható önaffin függvények segítségével.

Az önaffin függvényekre teljesül az alábbi tulajdonság

$$h(x_1, ..., x_n) = \lambda_1^{-\alpha_1} ... \lambda_n^{-\alpha_n} h(\lambda_1 x_1, ..., \lambda_n x_n),$$

ahol α_i durvulási vagy Hurst-kitevő. Tipikusan általában csak egy karakterisztikus durvulási kitevőnk van (α), és skálázás szempontjából az x_i értékek ekvivalensek, azaz egyszerűbben $h(x) = \lambda^{-\alpha} h(\lambda x)$. Belátható, hogy lokálisan az önaffin függvények Hölder folytonosak α exponenssel [2].

Az önaffin felületnövekedés dinamikáját egyrészt egyszerűsített rácsmodellek, másrészt a fizikai folyamat lényegét leíró egyenletek (sztochasztikus és determinisztikus parciális differenciálegyenletek — PDE) segítségével tanulmányozhatjuk.

A sztochasztikus felületnövekedést és a részecskék összetapadását szimuláló rácsmodellek megértését segítette elő az a programcsomagunk, amelyet 1992-ben a World Scientific kiadó publikált és terjesztett [6]. Megjelenésekor ez a maga nemében első ilyen programcsomag volt. Sikerrel használták elsőrban az oktatásban, esetenként kutatási feladatok megoldásában is. Rövid leírását a dolgozat függelékében adjuk meg.

A fent leírt fizikai folyamatok során kialakuló durvuló felület dinamikáját általában az alábbi Kardar-Parisi-Zhang (KPZ) egyenlettel lehet modellezni [13]:

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

Itt η többnyire nem korrelált zajt jelöl, ν a felületi feszültség, λ konstans. Az általunk vizsgált esetekben $(x, t) \in \mathbb{R}^2$, $h(x, t) \in \mathbb{R}$ a határfelület magassága (távolsága) az x helyen a t pillanatban, az eredetileg sima kezdeti felülettől ($h(x, 0) = 0$) mérve.

Vizsgálataink a fizika és a matematika határterületén mozognak, gyakran a számítástechnikát használva eszközül. Két fő irányra koncentráltunk.

1. Fizikai kísérletekhez kapcsolódó sztochasztikus növekedési modellek

Fizikai kísérletekhez kapcsolodó önaffin fraktálfelületek növekedését kívántuk modellezni. A kapott nemlineáris sztochasztikus differenciálegyenleteket numerikus szimuláció segítségével vizsgáltuk. A kísérleti és numerikusan kapott felületek összehasonlítására használt mennyiségi mutatók a skálázási exponensek. Ezek az exponensek a felület valamilyen fontos jellemzőjének (például a $w(t)$ felületszélességnek, vagy a $c(x,t)$ magasság-magasság korrelációs függvénynek) a viselkedését írják le.

A nedvesítési frontok kísérleti vizsgálatai során kapott eredmények [15],[16] nincsenek összhangban a KPZ egyenlet megoldásával. Ennek fő oka, hogy inhomogén közegben való terjedés leírásakor a fluktuációkat mint befagyott zajt kell figyelembe venni, szemben a KPZ egyenletben szereplő termikus típusú zajjal. (A befagyott $\eta(x,h)$ zaj nemlineárisan függ a felület magasságától, $h(x,t)$-től.) Új, a kísérleti eredményeknek jobban megfelelő modellt definiáltunk [27],[28]. A zaj multiplikatív módon szerepel ay egyenletben, mert ez az eset jobban megfelel a kísérleti körülményeknek, ha a felület anyagtranszport következtében mozog. A vizsgált egyenlet

$$\frac{\partial h}{\partial t} = \nabla^2 h + v[1 + (\nabla h)^2]^{1/2}(p + \eta),$$

ahol $p > 0$ konstans, v a sebesség felületre merőleges komponense és $\eta > 0$ a korrelálatlan befagyott zajnak felel meg.

Főbb eredményeink a fizikai kísérletekhez kapcsolódó modellben

A befagyott zaj a korábbiaktól eltérő, új skálázási exponenseket határoz meg. A numerikus integrálás eredményeként azt kaptuk, hogy a felület időbeli durvulását leíró β exponens értéke befagyott multiplikatív zaj esetében közel van 0.65-höz; ami

- (i) egyfelől rendkívül jó egyezésben van a kísérleti eredményekkel,
- (ii) másfelől lényegesen eltér a nem befagyott zaj esetére vonatkozó, az elméletből ismert 1/3-os értéktől;
- (iii) ezenkívül megfigyelhető, hogy az eredetileg egyenletes eloszlású input zaj hatványtörvénynek megfelelő eloszlású lesz a felület mentén.

2. Komplex téridő viselkedésű determinisztikus növekedési modellek

Az elmúlt néhány évben nyilvánvalóvá vált [24], hogy a d dimenziós komplex téridő–viselkedés érdekes megközelítési módjait kapjuk, ha az ott fellépő struktúrák leírására használt különböző függvényeket a $d+1$ dimenziós térben növekvő (durvuló) felületnek tekintjük. Ezeket a $d+1$ dimenziós felületeket pedig a fraktálgeometria terminológiájával, fraktálfüggvények segítségével leírhatjuk.

A komplex irányított polimerek elméletéből származó Zhang egyenletet [17] vizsgáltuk numerikusan és analitikusan

$$\frac{\partial h(x,t)}{\partial t} = \nabla^2 h(x,t) + \text{szingularis tag}$$

az alábbi szinguláris tagokkal

$$|\nabla h|^\alpha \qquad \alpha < 1 \qquad \text{vagy} \qquad \ln(|\nabla h|).$$

Ezt a zaj nélküli (determinisztikus PDE-vel leírt) komplex viselkedésű rendszert fizikusok és később matematikusok is tanulmányozták. Egyszerű alakja ellenére mindmáig nem teljesen feltárt a megoldás komplex viselkedése (egyáltalán létezése, stabilitása stb.).

- Numerikus vizsgálatok

  Úgy találtuk, hogy a nemlineáris vagy instabil PDE-k esetében a diszkretizáció szinguláris perturbációt jelent, tehát a numerikus megoldás során a folytonos egyenlet megoldásához képest egy minőségileg különböző megoldáscsalád kapható csak meg. A Zhang-egyenlet alábbi paraméteres változatait vizsgáltuk

$$\frac{\partial h}{\partial t} = \nabla^2 h - B \ln(|\nabla h| + A) \tag{4.1}$$

  és

$$\frac{\partial h}{\partial t} = \nabla^2 h + B|\nabla h + A|^\alpha. \tag{4.2}$$

  Itt $A > 0$ az egyes szimulációk alatt (kis) konstansként rögzített érték és B a szinguláris tag súlyát szabályozó paraméter.

  A kezdeti $h(x, 0)$ véletlen felület, amelynek magassága 0.0 és 0.01 közötti egyenletes eloszlású. A szimulációkban periodikus határfeltételeket használtunk.

Numerikus vizsgálataink fő eredményei

A B paraméter értékét változtatva a megoldás globális viselkedésének különböző érdekes átalakulásait — sztochasztikus és determinisztikus viselkedést (valamint azok keverékét) — sikerült megfigyelni és mennyiségileg leírni a (4.1) egyenletre és $\alpha < 0$ esetén a (4.2) egyenletre. [29].

A $B = 0$ esetben a felület teljesen kisimul ahogy $t \to \infty$. A (4.1) egyenletre a B értékét növelve ($A \leq 1$) a felület 'durvul' (3.5a ábra), míg $B > B_L$ esetén a felület adott meredekségű lineáris szakaszokból áll (3.5b ábra). Talán a legérdekesebb, ahogy a sztochasztikus viselkedés átvált determinisztikusba. Ekkor van egy váltakozó periódus, mikor a majdnem tökéletesen reguláris (szakaszonként) növekedést megszakítja a sztochasztikusan növekvő rész (3.5c ábra) vagy olyan átmenet is megfigyelhető, amelyben a későbbi stádiumban véletlenre váltó felület részei szakaszonként lineárisak miközben a felület többi része rendezetlen marad. A B paramétertől való függést jól meghatározható kitevőjű hatványtörvény írja le.

Az $\alpha > 0$ ($\alpha < 1$) eset teljesen különböző, mivel a szinguláris tag pozitív kitevővel nem divergál, amikor a gradiens nullához tart. Itt csak a két fő változat jelent meg a B paramétertől függően (lásd 3.10. ábra): durva fraktálfelület, illetve olyan felület, amelyen egyenes hullámszerű részek mozognak az x tengely mentén [30].

- **Az analitikus vizsgálatok eredménye**

  A paraméterek nélküli Zhang egyenlet logaritmus tagú változatát analitikusan vizsgálva sikerült speciális megoldásokat találni. A haladó hullám $h(x - \lambda t)$ és az önhasonló megoldás geometriai tulajdonságait vizsgálva bebizonyosodott, hogy a numerikus megoldás esetén látható struktúrák (hullámszerű, egyenes vonalakból álló részei) (lásd például 3.13. ábra) lokálisan úgy viselkednek, mint az általunk talált speciális megoldások (3.16. ábra) [31].

Appendix A

Fractal Growth software package

About two decades ago due to the activity of Benoit Mandelbrot, physicists (and later other scientists) became interested in fractals and the field was developing fast. It was realized that the rich variety of complicated patterns in nature can be successfully modelled by simple fractal growth models which capture the essential physics behind the associated phenomena. Computer simulations of such aggregation models have been playing an important role in our understanding of far-from-equilibrium growth processes. We developed a sofware package for the demonstrations of fractal aggregation models for IBM and compatible personal computers which was published in 1991 by World Scientific ([6]). Besides the diskette with the software it includes a user manual with short introduction about fractals and the models.

The program automatically detects the video standard of the particular configuration (available those years) and adjusts the model parameters accordingly.

The software is menu driven. The menus are organized hierarchically. Each time an item is selected a new level is entered (until the last level). The six menus are presented in the following Figures.

Different variants of four kinds of aggregation models have been presented: beside ballistic and Eden models (described briefly in Chapter 2), diffusion

limited aggregation and other models (cellular automaton, percolation, random walk). The user could choose from the menus even a short explanation of the particular model with the corresponding formulas and could learn a few tricks, e.g., how to simulate diffusion effectively.

The programs were developed using Turbo Pascal 5.5. They were compatible with higher versions (up to 7.0 we tested later). The names of the Pascal files and the corresponding models are

- BBUSH.PAS — Ballistic deposition on a single seed particle
- BDEP.PAS — Ballistic deposition onto a straight line
- CELL.PAS — Probabilistic cellular automaton (clouds)
- DLA.PAS — Diffusion limited aggregation (demo)
- DLA.PAS — Diffusion limited aggregation (faster version)
- EDEN.PAS — Eden growth around a seed particle
- EDENAV.PAS — Eden growth with noise reduction
- EDEP.PAS — Eden growth along a straight line
- PERCOL.PAS — Growing percolation
- RDEP.PAS — Random deposition
- WALK.PAS — Random walk on a plane

Our software package was unique since the Fractal Growth diskette contained the source files of the programs as well. It made possible for the user to learn and to design his or her own versions of the aggregation models. The package served both the educational purpose and research.

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