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Mathematical technology for solving the Kardar-Parisi-Zhang equation with a source

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Abstract. The description of an algorithm for numerical solution of the two-dimensional Kardar-Parisi-Zhang equation with fractal initial condition and spatially inhomogeneous stochastic source of particles has been presented. Using the Cole-Hopf substitution, the Kardar-Parisi-Zhang equation is reduced to an auxiliary linear parabolic equation with a variable coefficient. This reduction provides both compatibility of the algorithm with the concept of mathematical technology and possibility of its practical realization on supercomputer using the MPI parallel programming technology and the ROOT framework. The required profile of the evolving surface is restored by the inverse substitution by solving the auxiliary equation, Opportunity of estimation of its autocorrelation function and its spectral power density, as well as the time dynamics of Shannon surface information, have been discussed.

1. Introduction

One of the key questions under implementation of nanotechnologies into practice is the question about quality of the solid state surface. To clarify this question models for temporal evolution of crystal surface under different technological processes are required. One of these models is the Kardar-Parisi-Zhang (KPZ) equation, at present the KPZ-equation being the most popular phenomenological equation for modelling of crystal growth (see [1] and references therein). This equation was derived in paper [2] to describe the process of growth of the surface of a solid with epitaxial technology. In accordance with this paper the KPZ-equation looks as follows:

$$\frac{\partial h}{\partial t} = c + \frac{c}{2} \left[\left(\frac{\partial h}{\partial x}\right)^2 + \left(\frac{\partial h}{\partial y}\right)^2 \right] + \nu \left(\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} \right) + Q(x, y), \tag{1}$$

where $h(x, y, t)$ is the height of the surface under investigation, x and y are spatial Cartesian coordinates, c is the rate of growth and ν is coefficient of surface diffusion, function $Q(x, y)$ being additional source of sputtering substance in the vicinity of the surface [1].

Equation (1) ought to be provided by initial condition corresponding to initial shape of the surface under investigation:

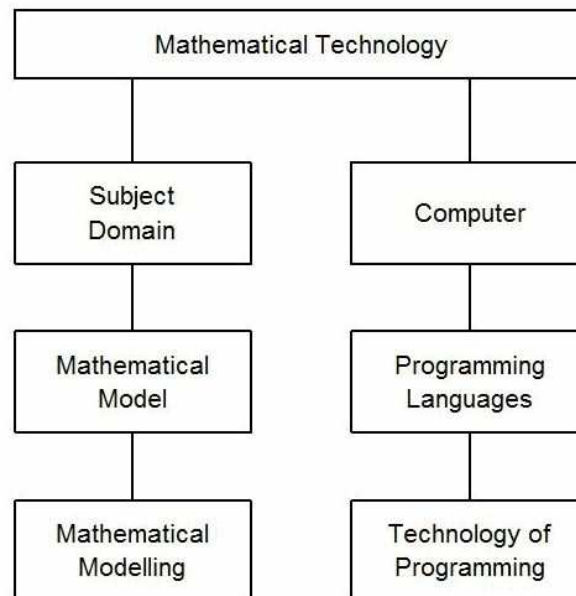$$h(x, y, 0) = h_0(x, y), \qquad (x, y) \in \Omega \subset R^2. \tag{2}$$

Figure 1. Structural scheme of mathematical technology concept

If $Q(x, y)$ is stochastic field then input equation (1) becomes stochastic partial differential equation.

There is a number of important values connected with solution of equation (1). The first of them is autocorrelation function of height:

$$K(\xi, \eta, t) = < (h(x, y, t) - < h(x, y, t) >)(h(x + \xi, y + \eta, t) - < h(x + \xi, y + \eta, t) >) >, \quad (3)$$

where angular brackets denote statistical averaging of function in them.

The two-dimensional spatial Fourier-transform from function (3) is known to be spectral power density of roughness of the surface:

$$S(p, q, t) = \int \int K(\xi, \eta, t) \exp(-i\, p\, \xi - i\, q\, \eta)\, d\xi d\eta. \quad (4)$$

Function (4) is significant because at every moment of time $t > 0$ it can be extracted from measurement of bistatic cross-section of monochromatic visible light with fixed polarization on this surface [3]. If λ is wavelength of this light source then for validity of this extraction the following inequality ought to be true [3]: $|h(x, y, t) - < h(x, y, t) > | \ll \lambda$. Other conditions for validity of this extraction namely $\left| \frac{\partial h(x,y,t)}{\partial x} \right| \ll 1$ and $\left| \frac{\partial h(x,y,t)}{\partial y} \right| \ll 1$ that is conjecture about small angles of the surface [3] coincide with conditions of validity for input equation (1) [2].

Another important value which can be constructed via the solution $h(x, y, t)$ of the Cauchy problem (1) and (2) is the Shannon information for the surface:

$$I(t) = \int_{\Omega} |h(x, y, t)| \log_2 |h(x, y, t)|\, dx dy. \quad (5)$$

At last often initial shape of the surface (2) proves to be fractal (see [4] and references therein). Moreover there is a variety of methods for estimation of fractal dimension D of network

approximation for function $h(x, y, t)$ [5]. And this value depends on time due to temporal evolution of the solid state surface in accordance with the KPZ-equation (1): $D = D(t)$.

Thus subject domain for the KPZ-equation (1) and values (3)-(5) connected to them is quite wide. It means that one ought to use under solution of this series of connected problems on supercomputer the concept of mathematical technology [6]. This concept includes two chains namely the first of them contains subject domain¡ mathematical models of considered subject domain and their mathenatical modelling and the second of them contains computer, programming languages and technology of programming (see Figure 1).

The rest of the article is organized as follows: in Section 2 we construct algorithm for numerical solution of the KPZ-equation (1). Section 3 deals with derivation of fractal initial shapes (2). In section 4 methods of numerical calculation of values (3)-(5) related to the KPZ-equation (1) are considered. In final section we summarize the results obtained and discuss perspectives of further investigations.

2. The algorithm for numerical solution of the KPZ-equation

Let us introduce a new unknown function $\varphi(x, y, t)$ as follows:

$$h(x, y, t) = c\,t + \frac{2\,\nu}{c}\,\ln \varphi(x, y, t)\,. \tag{6}$$

The expression (6) is known to be the Cole-Hopf substitution [2]. By means of this formula, one can reduce the nonlinear equation (1) to a linear parabolic equation with a variable coefficient:

$$\frac{\partial \varphi}{\partial t} = \nu \left(\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} \right) + \frac{c\,Q(x, y)}{2\,\nu}\,\varphi\,. \tag{7}$$

In accordance with (6) initial condition for equation (7) is equal to:

$$\varphi(x, y, 0) = \exp \left[\frac{h_0(x, y)}{2\,\nu} \right]\,, \qquad (x, y) \in \Omega \subset R^2\,. \tag{8}$$

To solve numerically the auxiliary linear Cauchy problem (7)-(8) at first let us suppose that domain Ω in (8) is a rectangular domain. Further one ought to segment the rectangular domain Ω into M rectangular subdomains Ω_m ($\bigcup_{m=1}^{M} \overline{\Omega}_m = \overline{\Omega}$) and to define on each Ω_m the simple problem in the framework of the method of fractional steps [7]:

$$\frac{\varphi_{ij}^{k+\frac{1}{2}} - \varphi_{ij}^{k}}{\tau/2} + \hat{\Lambda}_x\,\varphi_{ij}^{k+\frac{1}{2}} + \hat{\Lambda}_y\,\varphi_{ij}^{k} = \frac{c\,Q_{ij}}{2\,\nu}\,\varphi_{ij}^{k}\,, \tag{9}$$

$$\frac{\varphi_{ij}^{k+1} - \varphi_{ij}^{k+\frac{1}{2}}}{\tau/2} + \hat{\Lambda}_x\,\varphi_{ij}^{k+\frac{1}{2}} + \hat{\Lambda}_y\,\varphi_{ij}^{k+1} = \frac{c\,Q_{ij}}{2\,\nu}\,\varphi_{ij}^{k+\frac{1}{2}}\,, \tag{10}$$

where τ and Δ are steps on time and space respectively, φ_{ij}^{k} and Q_{ij} are network functions corresponding to continuous functions $\varphi(x, y, t)$ and $Q(x, y)$ and

$$\hat{\Lambda}_x\,\varphi_{ij}^{k} \equiv -\nu\,\frac{\varphi_{i+1,j}^{k} - 2\,\varphi_{ij}^{k} + \varphi_{i-1,j}^{k}}{\Delta^2}\,, \quad \hat{\Lambda}_y\,\varphi_{ij}^{k} \equiv -\nu\,\frac{\varphi_{i,j+1}^{k} - 2\,\varphi_{ij}^{k} + \varphi_{i,j-1}^{k}}{\Delta^2}\,.$$

To join solution of the simple problem (9)-(10) on subdomain Ω_m with solutions on neighboring subdomains one should impose exchange boundary conditions [6].

After that one can restore network function h_{ij}^{k} using discrete analog of formula (6).
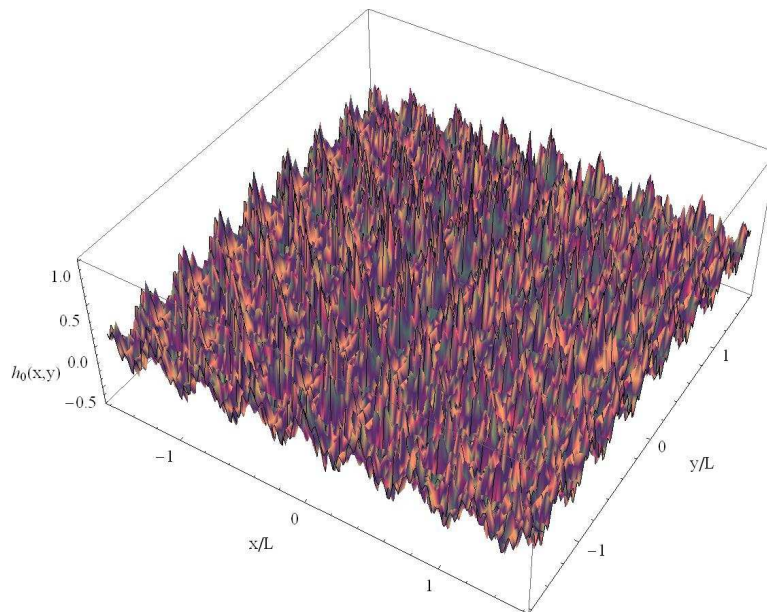
Figure 2. Regularized fractal initial shape

3. Regularization of fractal initial condition

Fractal functions are known to be nowhere differentiable (see [5] and references therein). For instance the well-known Weierstrass function

$$W(x, \vec{\mu}) = \sum_{n=1}^{\infty} a^n \cos \frac{\pi \, b^n \, x}{L} \,, \tag{11}$$

where $\vec{\mu} = (a, b, L)$ is vector of its parameters under $0 < a < 1$ and $a\,b > 1$ has no derivative but possesses by fractal dimension $D = 2 + \ln a / \ln b$ [5].

From function (11) it is easy to construct two-dimensional fractal surface:

$$W(x, y, \vec{\mu}) = W(x, \vec{\mu}) \, W(y, \vec{\mu}) \,. \tag{12}$$

On the other hand for parabolic equations existence and uniqueness theorems require that initial conditions (2) and (8) for the KPZ-equation (1) or auxiliary equation (7) must be quite smooth [8].

One can overcome this obstacle by means of some regularization of function (12) namely let us consider truncated Weierstrass function:

$$W_N(x, \vec{\mu}) = \sum_{n=1}^{N} a^n \cos \frac{\pi \, b^n x}{L} \,. \tag{13}$$

It is not difficult to check that direct product of functions (13) obeys to the next inequality:

$$|W(x, y, \vec{\mu}) - W_N(x, y, \vec{\mu})| \leq \frac{2 \, a^{N+2}}{(1-a)^2} \,, \tag{14}$$

where

$$W_N(x, y, \vec{\mu}) = W_N(x, \vec{\mu}) \, W_N(y, \vec{\mu}) \,. \tag{15}$$

Thus inequality (14) means that for any fixed accuracy smooth function (15) can approximate fractal function (12) under quite large number N of terms in sum (13) hence regularized fractal function (15) can be chosen as initial condition (2) $h_0(x, y)$ for the KPZ-equation (1). The result of such approximation under $a = 0.5$, $b = 5.0$ and $N = 11$ is presented on Figure 2.

It is obvious that the above described approach can be generalized on unequal numbers of terms and unequal vectors of parameters under taking direct product on x and y of truncated Weierstrass functions (13).

4. Estimation of values connected with the KPZ-equation

In order to calculate numerically autocorrelation function (3) it is necessary to describe a procedure for statistical averaging of different functions of height $h(x, y, t)$.

The most trivial algorithm of averaging is the following one. At first one ought to solve the simple problem (9)-(10) on each rectangular subdomain $\overline{\Omega}_m$ for different realizations of source $Q_\alpha(x, y)$, $\alpha = 1, 2, \ldots, A$. After that average value of function f is equal to:

$$< f >= \frac{1}{A} \sum_{\alpha=1}^{A} f_\alpha,\tag{16}$$

where value f_α corresponds to realization $Q_\alpha(x, y)$.

Further spectral power density of roughness of the surface (4) it is convenient to estimate as discrete Fourier transform because of there are parallel algorithms to perform this operation [9].

The Shannon information for the surface (5) is additive function of domain Ω:

$$I(t) = \sum_{m=1}^{M} I_m(t),\tag{17}$$

where

$$I_m(t) = \int_{\Omega_m} |h(x, y, t)| \log_2 |h(x, y, t)| \, dx dy.\tag{18}$$

To calculate integrals (18) on the basis of network functions φ_{ij}^k one ought to use different cubature formulae [10].

In addition, a triple autocovariation function can be calculated on individual lines as a characteristic of the non-Gaussianity of the process.

5. Conclusion

This article presents the algorithm of numerical solution of the two-dimensional KPZ-equation with a time-independent random surface source of particles and a regularized fractal initial condition adjusted to the concept of mathematical technology [6]. Such a reanimation of the concept of mathematical technology is currently extremely relevant in anticipation of the emergence of supercomputer exaflop performance [11].

This algorithm is expected to be realized on the Lomonosov supercomputer [12] using the MPI parallel programming technology and the ROOT object oriented data analysis framework [9].

The elaborated algorithm is very important for practice because of the study of the properties of solutions of the KPZ-equation is essential for understanding the processes of nanoengineering [13].

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