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Determination of the Kardar–Parisi–Zhang equation from experimental data with a small number of configurations

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HIGHLIGHTS

- Inverse method to determine the parameters of the KPZ equation.
- The approach requires few interfaces as input data to perform the modeling.
- The approach is applied to a stochastic cellular automata and an RSOS model.

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ABSTRACT

We introduce an inverse method to determine the parameters of the Kardar–Parisi–Zhang equation corresponding to an evolving interface which requires a small number of configurations as input data. Our approach presents advantages for applications in real world scenarios since it does not require small time intervals between fronts. The method is applied to a restricted solid-on-solid model and a stochastic cellular automata model for fire front propagation.

1. Introduction

Surface fire spread remains a challenging problem associated to kinetic roughening, which is also present in crystallization front growth, material deposition, corrosion on a substrate, tumor expansion, and fluid flow in porous media [1–3]. The dynamics of these models can be represented by a moving interface, and particularly experiments on fire front propagation in paper sheets [4–8] indicate that it can be modeled by the Kardar–Parisi–Zhang (KPZ) equation [9]:

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

describing the local growth rate of an interface height $h(x,t)$, where ν and λ are the diffusion coefficient and nonlinear parameter, respectively, and c is related to the average growth rate. The noise term η has a Gaussian distribution with $\langle\eta(x,t)\rangle = 0$ and $\langle\eta(x,t)\eta(x',t')\rangle = 2D\delta(x-x')\delta(t-t')$, where $\langle\cdots\rangle$ stands for an ensemble average.

The correct determination of the equation describing experimental data is guided by the knowledge of the universality class of the process, and some approaches can be used for this purpose [5]. Determining scaling exponents allows us to compare them with those obtained analytically or numerically from known models [4]. Some discrete models such as the

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restricted solid-on-solid (RSOS) model [10,11] and the ballistic deposition (BD) model [1,12] are known to be described by the KPZ equation in the continuum limit. Starting from a master equation for the configuration probability, the discrete Langevin equation is obtained and the continuous limit is determined by regularization techniques [13–16]. Ref. [17] introduces a coarse-grained approach using test functions to compute the linear and nonlinear coefficients applying tilt transformations on the average velocity [1,18,19]. However both approaches require the specification of the transition rate, which is not always known for empirical systems.

The parameters in the KPZ equation can be determined from experimental or simulation data given by a set of fronts by using an inverse method. Lam and Sander [20] presented an approach that consists in computing the derivatives $\partial h/\partial t$, $\nabla^2 h$ and ∇h in Eq. (1) from the experimental data and then minimizing the deviation function $\mathcal{D} = \langle[\partial h/\partial t - c - \nu\nabla^2 h - \lambda/2 (\nabla h)^2]^2\rangle$ with respect to c, ν and λ. As a consequence short time intervals separating experimental fronts are required to compute the time derivative. Here we propose a new approach that can be implemented for any number of interfaces for modeling, even if they are widely spaced in time. Our approach is illustrated with applications to a restricted solid-on-solid model and a fire propagation model based on stochastic cellular automata.

The structure of the paper is as follows: Section 2 discusses how to determine the universality class from experimental data. Section 3 shortly presents the numerical scheme for the integration of the KPZ equation and Section 4 presents our approach for the determination of the coefficients in this equation. Section 5 presents the application of the approach to the RSOS and stochastic cellular automata models. We conclude the paper with some concluding remarks in Section 6.

2. KPZ universality class

The interface width characterizing the roughness of the interface is defined as the rms fluctuation of the height [1]:

$$w(L,t) \equiv \left\langle \left[\frac{1}{L} \sum_{i=1}^{L} [h_i(t) - \bar{h}(t)]^2 \right]^{1/2} \right\rangle, \tag{2}$$

where $h_i(t)$ is the interface height at time t of the ith column on a substrate of length L, the angular brackets denote a configurational average and $\bar{h}(t)$ denotes a spatial average. For shorter times it scales as [1]:

$$w(L,t) \sim t^{\beta}, \quad t \ll t_{\times}, \tag{3}$$

where $t_{\times}$ is the crossover time to a saturated regime and β is the growth exponent characterizing the time-dependent dynamics of the roughening process. For longer times the interface reaches saturation values w_{sat} that scales as a power law of the system size L [1]:

$$w_{\mathrm{sat}}(L) \sim L^{\alpha}, \quad t \gg t_{\times}, \tag{4}$$

where α is the roughness exponent. Theoretical predictions [1,3,4,9] based on analytical calculations and computer simulations show that fronts from interface growth are self-affine fractals with $\alpha = 1/2$ and $\beta = 1/3$ in $d = 1 + 1$ dimensions.

Different methods to determine the universality class from experimental data are described in the literature [3,4,7,11,21–23]. Alternatively and independently the scaling exponents can be estimated using the height–height correlation function [1,4]:

$$C(\zeta, \tau) = \left\langle [\delta h(x+\zeta, t+\tau) - \delta h(x,t)]^2 \right\rangle_{x,t}, \tag{5}$$

where $\delta h \equiv h - \bar{h}$ and the brackets $\langle \cdots \rangle_{x,t}$ denote temporal, spatial and ensemble averages. The roughness exponent can be determined from the relation $C(\zeta, 0) \sim \zeta^{2\alpha}$ up to the parallel correlation length of the system. The growth exponent can be determined from time delayed correlations as $C(0, \tau) \sim \tau^{2\beta}$ for times shorter than $t_{\times}$.

3. Numerical integration of the KPZ equation

Different methods for the numerical solution of the KPZ equation are presented in the literature [24–30], and any can in principle be used in the present approach. The KPZ equation (1) in $1 + 1$ dimensions is discretized as:

$$\frac{\mathrm{d}h_i(t)}{\mathrm{d}t} = c + \frac{1}{\Delta x^2} \left[\nu \Gamma_i + \frac{\lambda}{2} \Psi_i \right] + \eta_i(t), \tag{6}$$

where $h_i(t)$ is the interface height at the ith cell of the lattice ($i = 1, \ldots, L$) at time t and Δx is the spatial resolution of the numerical grid. The standard choice for the diffusive term is

$$\Gamma_i = h_{i+1} + h_{i-1} - 2h_i. \tag{7}$$

The nonlinear term in Eq. (6) admits different discretizations [25,29]:

$$\Psi_i^{(\gamma)} = \frac{1}{2(\gamma+1)} \left[(h_{i+1} - h_i)^2 + 2\gamma (h_{i+1} - h_i)(h_i - h_{i-1}) + (h_i - h_{i-1})^2 \right]. \tag{8}$$