Lattice Model for Approximate Self-Affine Soil Profiles

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Abstract

A modeling of the soil structure and surface roughness by means of the concepts of the fractal growth is presented. Two parameters are used to control the model: the fragmentation dimension, $D_f$, and the maximum mass of the deposited aggregates, $M_{\text{max}}$. The fragmentation dimension is related to the particle size distribution through the relation $N(r \geq R) \sim R^{D_f}$, where $N(r \geq R)$ is the accumulative number of particles with radius greater than $R$. The size of the deposited aggregates are chose following the power law above, and the morphology of the aggregate is random selected using a bond percolation algorithm. The deposition rules are the same used in the model of solid-on-solid deposition with surface relaxation. A comparison of the model with real data shows that the Hurst exponent, $H$, measured \textit{via} semivariogram method and detrended fluctuation analysis, agrees in statistical sense with the simulated profiles.

Key words: surface roughness, soil modelling, self-affine profiles
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1 Introduction

The concepts of the fractal geometry have been widely used to describe and quantify irregularity in nature, and statistical self-affine properties have recently been identified in various Earth’s terrain [1] and profiles [2]. Several works in soil science incorporates the fractal geometry to describe and modeling soil physical properties, soil physical processes and quantify the soil spatial variability [3–6].

A very important property closely related to the fractal geometry is the soil surface roughness, defined as the configuration of the soil microrelief. The soil surface roughness exerts great influence on water infiltration, erosion and run-off effects. Its quantification is important for understanding the soil behavior during degradation processes like rainfall erosion or abrupt changes such as those induced by tillage [7]. In the last years, a considerable effort was done to simulate the soil structure; several models propose the simulation of the particle size distributions [4], the soil surface roughness [3,8], the morphology of the pore-solid structure [9], etc. The major properties considered in these models are the fractal dimension of the soil surface, $D$, the particle size distribution (PSD), the pore size distribution and the surface roughness.

In this work we present a simple lattice model to simulate the soil structure and reproduce the surface soil roughness. We basically use the ideas of the fractal growth models [10] to generate an approximate self-affine profile, that exhibit, as much as possible, a similitude with the fractal properties of real soils. It is approximate in the sense that the scaling properties of these profiles are valid only in a limited range of scales. Therefore, the model was validated by means of a comparison between the fractal dimension estimated for simulated profiles and for natural soil surfaces. The major improvements in our model are the power law distribution of the sizes of the deposited particles or aggregates and a random selection in the allowed morphologies of the aggregates. This two features, not improved before by any model, are responsible for the soil structure in our model. In the section II we present a detailed description of the model, showing the particle size distribution and explaining the algorithm for the random choice of the morphologies. We also present a brief summary of the theory of growth surfaces. In the section III is presented the results for several maximum aggregates sizes and different fragmentation dimensions. Finally, in the section IV we present our conclusions and perspectives.
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\( R = \sqrt{\frac{M_{\text{max}}}{\pi}} \)

10

10

1

2

3

4

5

\( N(r > R) \)

Fig. 1. Particle size distribution for a simulated soil with \( M_{\text{max}} = 1000 \) and \( D_f = 3.0 \). The radius of the particles are calculated via the expression: \( r^2 = \frac{M}{\pi} \), that approximates the particles by discs with area \( M \). Note the power law behavior for the particles sizes.

2 The Model

The motivation in elaborate this model lies in aptitude to simulate some of the majors properties of agricultural soil, like self-affine profiles and porous medium. The model have to allow the possibility to change some parameters, as the aggregate size distribution, and the maximum mass of the aggregates. These two parameters try to cover the structural variability found in natural soils. The aggregate size distribution is assumed to have power law behavior \([5,6]\), and their exponent, \( D_f \), is one of the parameters of the model. The other parameter, \( M_{\text{max}} \), is the maximum mass of particles utilized to generate the aggregate, which is approximately related with the square of maximum aggregate radius. In spite of others classical lattice models, where the particles generated always have the same morphology, this model simulate the variability observed in natural soil, generating aggregates by a bond percolation algorithm. All this characteristics have to be integrated in a very simple model to allow the simulation of relatively large systems (\( L = 1000 \)).

In this way, the major improvement to choose a lattice model is the simplicity and the velocity to run the code, what possibilities the simulation of large systems with great quantity of deposited particles (hundred millions). This massive number of deposited particles are needed in order to avoid the effect of the constant attachment of micro random variability, represented by the random morphology of the aggregates. Another advantage to work in the lattice, is the theoretical background furnished by the fractal growth theory, presented by Barabási and Stanley [10].

We consider the soil structure composed by a set of particles and aggregates whose radius are power law distributed according to the following relation,
known as Turcotte’s empirical law [5],

\[ N(r > R) \sim R^{-D_f}, \]  

(1)

where \( N(r > R) \) is the cumulative number of particles (or aggregates) with radius \( r \) greater than \( R \) and \( D_f \) is the fragmentation dimension of the particle size distribution (PSD). There is some controversy in the literature about the allowed range of the values of the \( D_f \). Tyler & Wheatcraft [11] argued that \( D_f < 3 \) because, under usual hypothesis (constant density, spherical particles, etc), the mass distribution scales with \( M(r > R) \sim R^D \sim R^{3-D_f} \), where \( D \) is the fractal dimension of the soil. Thus, considering a fractal distribution, only the values \( D_f < 3 \) have physical meaning. Martin & Taguas [4] present several mathematical arguments supporting this conjecture, and show some PSD simulations. However, there are several experimental studies, summarized by Perfect & Kay [5] where the range of values of \( D_f \) is \( 2.6 < D_f < 3.5 \). Gimenez et al [12] also affirm that there is not any experimental relation between the fractal dimension and the fragmentation dimension. We consider that the usual hypothesis of constant density of the particles is not valid when the radius of the aggregates grows up, due the presence of pores in the structure. Thus, fragmentation dimensions greater than 3 are, in principle, allowed.

According to the USDA classification of soil texture [13], the basic particle size classification is:

- sand \( 50 < r < 2000 \mu m \)
- silt \( 2 < r < 50 \mu m \)
- clay \( r < 2 \mu m \).

The real soils can vary widely in the percentile of each range of sizes. The study of Nemes et al proposes a standardisation of the classification of the European soils and shows several experimental data [13]. In the figure 1, we present a typical PSD generated by the algorithm of the model. This PSD is constructed considering that the particles are approximately circles; so, there is a direct relationship between the mass number and the particle radius, that is used to build the PSD.

The model has two parameters, the fragmentation dimension, \( D_f \), and the maximum mass of the aggregates, \( M_{max} \). To every particle is selected a mass number, \( M \); when \( M > 1 \), the model choose a random configuration for it; this choice is one of the possible bond percolation clusters with a given size. In the figure 2, we show some of the possible aggregate morphologies. These two parameters try to cover, in a simple way, the structural variability found in natural soils.

The deposit of each particle follows the model of the solid-on-solid deposition with surface relaxation [10]. The initial position for the deposition is random.
Fig. 2. A) Possible morphologies for $M = 4$. In this case, the morphologies are the same observed in a popular game called “Tetris”. B) Some morphologies for $M = 400$. Three morphologies are shown. Note the porous structure of the aggregates, and its random shape. C) Soils profiles generated by the model. Above: typical deposition in a lattice with $L = 200$, 20000 particles deposited with $M_{\text{max}} = 100$ and $D_f = 3.0$. Below: the same, with $D_f = 2.0$. Note the variability of the soil structure with the fragmentation dimension.

chose and the particle follows a straight line until touch the soil surface. Then, the algorithm simulate a surface relaxation (without rotation) to the particles, which only are adhered to the bulk when they reach the site with the local minimum energy.

Considering the theory of growth surfaces, the solid-on-solid deposition belongs to the universality class of the Edwards-Wilkinson equation

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

(2)

where $h(x,t)$ is the height of the site $x$ at time $t$, and $\eta(x,t)$ represents a random noise, that expresses the fluctuations in the arrive of the particles and had the following properties, $\langle \eta(x,t) \rangle = 0$ and $\langle \eta(x,t) \eta(x',t') \rangle = 2C \delta^d(x-x') \delta(t-t')$. The $\delta$ is the usual Kronecker delta and $C$ is a diffusion constant.

The width of the growth surfaces, $w(L,t)$ then obeys a scaling relation

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

(3)

where $f(u)$ is a scaling function: $f(u) \sim u^\beta$ for $u << 1$ and $f(u)$ is a constant for $u >> 1$; $\alpha$, $\beta$ and $z$ are the roughness, the growth and the dynamical exponents, respectively. They are known as the scaling exponents and are
Fig. 3. Roughness of the simulated profiles, with several $M_{\text{max}}$ and $D_f = 3.0$. Note the variation of the slope between the two vertical dotted lines, shown in the small window. The slope is measured with a rule with fixed length, and varies the initial point since the left vertical line to the right.

related by the scaling law

$$z = \frac{\alpha}{\beta}. $$

The EW scaling exponents are known exactly: $\alpha = 1/2$, $z = 2$.

Another equation related to the deposition is the Kardar-Parisi-Zhang equation, that has a nonlinear term,

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

(4)

To this equation the calculated exponents are $\alpha = 1/2$, $z = 3/2$.

So, we perform simulations to test the influence of the model parameters $D_f$ and $M_{\text{max}}$ in the scaling exponents and fractal dimension of the soil profiles, and compare the results with the experimental data disposable.

3 Results

We perform simulations in one dimensional lattice with length $L = 1000$ sites. The results for the scaling exponents represent the average value in a set of 20 samples with the same parameters in each simulation, and different deposition sequence of the random aggregates. The number of particles/aggregates
deposited in each sample is $N = 100000000$. The behavior of the local width, $w(L, T)$, defined by

$$w^2(L, t) = \frac{1}{L} \sum_{i=1}^{L} \left( h_i(t) - \overline{h}(t) \right)^2 ,$$

(5)

with the model parameters are shown in the figure 3. Note the roughness saturation at $N \sim 10000000$. The fractal dimension of the final profile is estimated using the Hurst exponent $H$. The Hurst exponent is associated to the fractal dimension via the relation $D = 2 - H$. There are several ways to measure $H$. At this work, we use the detrended fluctuation analysis (DFA), improved by the first time by Moreira et al [15], and the semivariogram method, that uses a height-height correlation function.

The DFA consists in measure the roughness around the mean square straight line [15]. The roughness $W(L, \epsilon, t)$ at the scale $\epsilon$, is given by

$$W(L, \epsilon, t) = \frac{1}{L} \sum_{i=1}^{L} w_i(\epsilon, t)$$

(6)

and the local roughness $w_i(\epsilon, t)$ is defined by

$$w_i^2(\epsilon, t) = \frac{1}{2\epsilon + 1} \sum_{j=i-\epsilon}^{j=i+\epsilon} \left\{ h_j(t) - [a_i(\epsilon)x_j + b_j(\epsilon)] \right\}^2$$

(7)

where $a_i(\epsilon)$ and $b_i(\epsilon)$ are the linear fitting coefficients to the displacement data on the interval $[i-\epsilon, i+\epsilon]$ centered at the site $i$. Self affine profiles satisfy the scaling law

$$W(\epsilon) \sim \epsilon^H$$

(8)

that is used to measure $H$. The semivariogram method estimates the spatial variability, through the calculus of the semivariance as a function of the distance between points. This function is can be estimated by:

$$\gamma(\epsilon, t) = \frac{1}{2n(\epsilon)} \sum_{i=1}^{n(\epsilon)} [h_i(t) - h_{i+\epsilon}(t)]^2 ,$$

(9)

where $h_i(t)$ the height in the location $i$ at time $t$, and $n(\epsilon)$ represents the number of pairs of points which are separated by $\epsilon$. In the case of self-affine profiles $\gamma$ exhibit a power law behavior,

$$\gamma(\epsilon) \sim \epsilon^{2H} ,$$
Fig. 4. Summary of the exponent values. A) and C): Behavior of the Hurst exponent with the model parameters. Note that there is not a remarkable trend to the Hurst exponent with any model parameters. The range of experimental values is $0.3 < H < 0.7$. B) and D): Behavior of the growth exponent with the model parameters. Note the dependence of the growth exponent with the average radius size: as the radius increase, the growth exponent increases too. The dependence of $\beta$ with the fragmentation dimension is inverse.

and, in the same manner as in the DFA method, the $H$ exponent can be utilized to calculate the fractal dimension.

The semivariogram method is especially useful in cases where the data are not regular spaced, and for this reason, is widely used in estimating fractal dimension of soil surfaces [5].

The range of the $H$ values is shown in the figure 4A and 4B. In the figure 4C and 4D, we show the dependence of the growth exponent with the model parameters. We conclude that the increase of the maximum particle mass $M_{\text{max}}$ have similar effects to the decrease of the fragmentation dimension: both introduces a nonlinear correlation in the system, expressed by the increase in the value of the growth exponent $\beta$, changing the universality class of the deposition. Nevertheless, the fractal dimension of the surface do not alters considerably with the model parameters.

4 Conclusions and Perspectives

In this work, we present a new model to simulate the soil structure and its surface roughness. Two parameters are used to control the simulated profiles: the maximum mass of the particles and the fragmentation dimension. The major improvements of this model are: the random configuration allowed to the particles or aggregates and the power law distribution of its radius. These two features are not present in any model discussed in the literature until to-
day, and permits the reproduction of the variability observed in natural soils. The results obtained shows a good agreement for the exponent $H$ calculated from the simulations and measured experimentally [7]. We also observe a dependence of the growth exponent $\beta$ with the maximum mass allowed to the particles: as the $M_{\text{max}}$ grows, the value of the $\beta$ exponent grows from the EW value ($\beta = 1/4$) to the KPZ value ($\beta = 1/3$). So, the increase of the averaged particle radius corresponds to the introduction of nonlinear correlations into the system.

Next, we expect increase the system size and control better the shape of the deposited particles, in order to perform simulations closer to the real soils. We also intend simulate the rainfall effect over the simulated structure, to verify the dependence of the Hurst exponent with the rain [14].

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