Monte Carlo fixed scale transformation for nonlocal fractal growth models

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The fixed scale transformation (FST) is a theoretical framework developed for the evaluation of scaling dimensions in a vast class of complex systems showing fractal geometric correlations. For models with long range interactions, such as Laplacian growth models, the identification by analytical methods of the transformation's basic elements is a very difficult task. Here we present a Monte Carlo renormalization approach which allows the direct numerical evaluation of the FST transfer matrix, overcoming the usual problems of analytical and numerical treatments. The scheme is explicitly applied to the diffusion limited aggregation case where a scale invariant regime is identified and the fractal dimension is computed. The Monte Carlo FST represents an alternative tool which can be easily generalized to other fractal growth models with nonlocal interactions. [S1063-651X(96)02512-3]

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The fixed scale transformation (FST) is a powerful analytical tool for the calculation of the fractal dimension of a variety of equilibrium and nonequilibrium models [1]. The practical implementation of this scheme is rather simple in standard critical phenomena, such as percolation, which are governed by local interactions. On the contrary, for fractal growth problems like diffusion limited aggregation (DLA) [2,3], both the matrix elements and the scale invariant dynamics analytical calculations represent a basic problem. For DLA the FST calculation has been carried out in its full extent, giving results in very good agreement with numerical simulations [1]. In general, however, given a growth model with long range interactions, the analytical evaluation of the scale invariant matrix elements is a formidable task [4–6].

For this reason, we show here a Monte Carlo (MC) procedure which deals directly with the FST transfer matrix elements. We develop a procedure for the numerical calculation of the scale invariant FST matrix elements, which finally yields the calculation of the fractal dimension. This Monte Carlo FST (MCFST) scheme allows us to overcome the problems arising in the analytical evaluation of the scale invariant dynamics. On the other hand, the Monte Carlo part of the method deals with local configuration calculations avoiding the usual numerical uncertainties given by the large scale corrections to scaling present in these models.

We apply explicitly this scheme to the DLA model. In order to do that we used numerically generated DLA clusters with size ranging from $L=128$ to $L=512$. On these clusters we numerically calculated the FST matrix elements for different coarse graining sizes. We find that the FST matrix elements approach a scale invariant regime. In this scale invariant regime we can easily compute the fractal dimension for DLA clusters, obtaining results in good agreement with the expected value. The MCFST is therefore a good alternative calculation scheme for models in which an analytical computation of the scale invariant dynamics is not yet achieved.

The FST approach starts with the full description of the nearest-neighbor pair correlations, and then uses the scale invariant dynamics to extract from them the scaling properties characterizing correlations at arbitrary scales. Let us first discuss the calculation at a given scale. In this respect it is convenient to consider the transverse correlations along the intersections of the structure with a line perpendicular to the local growth direction. In two dimensions, since we are interested in conditional probabilities, there are two types of pair configurations in the asymptotic structure. A configuration of type 1 consisting of an occupied site and an empty one, and a type 2 with both sites occupied. The occurrence probabilities of these configurations are defined as C_1 and C_2, respectively. In order to compute these probabilities we consider the probabilities $M_{i,j}$ that a pair configuration of type i is followed in the growth direction by a configuration of type j. These conditional probabilities leads to the following transfer matrix problems:

$$\begin{aligned} C_1^{k+1} &= M_{1,1}^k C_1^k + M_{2,1}^k C_2^k \\ C_2^{k+1} &= M_{1,2}^k C_1^k + M_{2,2}^k C_2^k, \end{aligned} \tag{1}$$

where the index k refers to different intersections of the structure. This is the FST matrix in its general formulation. Because of the translational invariance of the structures considered [7], the transfer matrix fixed point (C_1^*, C_2^*) characterizes nearest-neighbor correlations at the same scale to which the dynamics used in the calculation is referred. The matrix elements $M_{i,j}$ can be computed by lattice path integrals over the possible growth processes that correspond to the configurations i and j. Therefore one must, in principle, consider all the possible series of growth processes with a statistical weight given by the growth rule of the model considered. The general scheme for the analytical calculation of the matrix elements is given in Ref. [1].

The above framework is very powerful because the use of the scale invariant dynamics in the FST calculation allows us to interpret sites as coarse grained cells. Therefore the fixed point probabilities (C_1^*, C_2^*) characterize geometrical correlations for coarse grained cells of any size. This corresponds

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to extract the fractal dimension from the large scale limit of the pair correlation function which is described by nearest-neighbor pair correlation of very large cells. In such a situation the probability distribution (C_1^*, C_2^*) can be related to the fractal dimension D_f of the structure [1], finally obtaining

$$D_f = 1 + \frac{\ln\left(\frac{2M_{1,2}+M_{2,1}}{M_{1,2}+M_{2,1}}\right)}{\ln 2}. \tag{2}$$

The scale invariant dynamical growth rules are therefore necessary for a complete definition of the FST approach. The knowledge of this scale invariant dynamics is also one of the key points in the understanding of why growth models give rise to fractal structures. For DLA we are in the position to understand some general properties of the scale invariant dynamics [4]. In addition it is possible to show with renormalization methods that the scale invariant dynamics is very close to the microscopic one from which the model is defined [5]. However a general understanding of the scale invariant dynamical regime for nonlocal growth models has not yet been achieved. In fact, for these models, the matrix elements calculation as well as the analytical form of the asymptotic dynamics, are very complex problems. By contrast, the standard MC approach of directly simulating the model of interest is very easy to apply and gives good results for the properties of finite systems [3]. However, when an attempt is made to calculate the properties of an infinite system, it runs into problems of finite size effects. In fact, the long range correlated dynamics in space and time of fractal growth problems, makes that scaling corrections decay extremely slow and in a nontrivial way.

To pursue a practical way of avoiding the difficulties of both the FST analytical calculation and the MC computer simulations, we combine the two methods to obtain a general and easily implemented computational scheme. We use a MC simulation to generate several cluster realizations of the growth model considered. Since the explicit configurations are stored in the computer, any function of interest can be calculated from these clusters. We then focus directly on the definition of the FST matrix elements. We perform a box covering of the cluster with boxes of size $\ell \times \ell$. At this point an opportune spanning condition or majority rule is chosen in order to decide which boxes can be considered occupied by the cluster. This step corresponds to define a coarse graining with scale factor ℓ. The next step is the study of intersections perpendicular to the growth direction. We consider pairs of $\ell \times \ell$ boxes on consecutive intersections. As shown above there are two types of pair configurations: a configuration of type 1 consisting of an occupied site and an empty one, and a type 2 with both sites occupied. The MCFST matrix elements $\mathcal{M}_{i,j}(\ell)$ are thus given by the normalized occurrence of local configurations in which a pair configuration of type i is followed on the next intersection by a pair configuration of type j. Given a MC simulation of size L, we can define on each intersection $(L/2\ell)$ pairs configurations of boxes, and we can look at $(L/2\ell)$ pairs of consecutive intersections. This gives $N \sim (L/2\ell)^2$ local configurations for the matrix elements statistics. We also have to look at the scaling of the FST matrix by performing different coarse graining steps for different box sizes ℓ. For self-similar systems the matrix elements have to approach a scale invariant regime in the range $1 \ll \ell \ll L$; i.e., $\mathcal{M}_{i,j}$ becomes independent from ℓ. This is the regime in which the FST calculations give the right value for the fractal dimension.

The MCFST scheme defined above does not involve the truncations usually involved in analytical calculations, and it is implicitly defined by the correct scale invariant dynamics. At the same time, the MC computational part is focused directly onto the local configurations of interest, avoiding the errors deriving by extrapolating large scale behavior. In the MCFST there are no approximations other than the coarse graining definition and the statistical uncertainty implicit in using finite cluster simulations. It is, however, worth stressing that there are several technical aspects of MC computer simulations that are extremely important in obtaining reliable numbers. Binder and Herrmann [8] have provided a detailed discussion of these essential points. The strategy we outlined retains also the advantage of being applicable to a large class of fractal growth models as well as equilibrium models. It is also interesting to note that a preliminary attempt to use such a technique can be found in [9], where a similar approach was used on percolation clusters.

To illustrate how MCFST calculations work in practice, we shall discuss the explicit application to the DLA model in two dimensions. DLA has been extensively investigated both numerically and theoretically [3] in the last decade. In addition, the analytical FST approach has been applied in its full extension to the two dimensional case [1,5,14]. This allows us to compare the results obtained in the present MCFST study with those obtained with other methods.

The basic DLA model is defined on a two dimensional square lattice [2]. The construction of DLA clusters begins with a particle at a random location on a ''birth'' region at some distance from the existing cluster. The new particle undergoes a Brownian motion until it comes in contact with the cluster, at which point it becomes permanently stuck. A new particle is then added at random and the process continues. One can define the growth process starting from a base line (the seed) and proceeding towards a faraway upper boundary line. Since, in practice, the length of the base line is finite and one uses periodic boundary conditions, topologically the growth occurs on the surface of a cylinder [10]. For this geometry the initial stage of growth (the scaling regime) shows the development of larger and larger correlations. When correlations reach the size of the basis the cluster enters the ''steady-state'' regime in which fractal properties are asymptotically defined. Here we use on-lattice cylindrical clusters with basis size ranging from $L=128$ to $L=512$. Each cluster was grown up to a height $h=4L$ to obtain a better statistics of the steady-state region. For each system size we averaged data over 10 realizations.

The first step of the MCFST consists in the implementation of a coarse graining procedure which defines the occupied boxes of size ℓ. By executing a covering of the DLA clusters we must in fact choose a criterion to decide when a cell can be considered occupied or not. A crucial point in the renormalization of growing structures is the preservation of the connectivity. In fact, at a generic scale, we have a growth event only if a cell is completely spanned by the growing structure. A similar problem is found in percolation, where

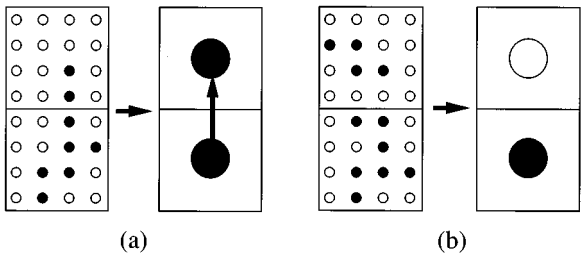

FIG. 1. Rescaling with the spanning rule. (a) The lower box is spanned, and the upper one is connected to the lower one. The two boxes both renormalize in an occupied site. (b) The lower box is spanned (black), while the upper one is neither spanned nor connected to the other one (white).

connectivity plays a fundamental role because it determines the critical state. We therefore consider only those cells spanned either from left to right or top to bottom, or cells which are connected to a spanned one. This spanning rule implies that only structures extending over the size of the rescaling length contribute to the renormalized cluster. Moreover, it ensures the connectivity properties of the cluster in the renormalization procedure.

To check the spanning of a cell of size ℓ we used a pattern-recognition algorithm, which looks for the branch connecting two opposite sides of the cell. The basic idea of this algorithm is to assign a label, a ''color,'' to the points in the cell, in such a way as points belonging to the same branch of the structure have the same color, each branch being characterized by a different color. To do so in our MCFST approach, we used the Hoshen-Kopelman algorithm [11,12] which gives to all connected sites in a cell the same label P (or ''color''). After having labeled all disconnected branches in a cell, it is sufficient to check if the same label appears in both the two sides of the cell, in order that the spanning condition be satisfied. In Figs. 1(a) and (b) we show two typical situations. In Fig. 1(a) we have two nearest neighbor 4×4 boxes; the lower one is spanned by a connected path, while the other is connected to the spanned one. The two boxes both renormalize in a site belonging to the structure. In Fig. 1(b), instead, the lower box is spanned, and the upper box is neither spanned nor connected to the lower one. So, the upper box renormalizes in an occupied site and the other renormalizes in an empty site.

After the coarse grained clusters at scale ℓ are defined, one computes the FST matrix elements $\mathcal{M}_{i,j}(\ell)$ as the normalized number of configurations of type i on the first intersection followed by a configuration of type j. We ignore configurations where pairs of white sites or diagonally connected black sites appear. The analysis is repeated for all intersections on the structure, different cluster sizes L and different coarse graining scales ℓ. In Fig. 2 the FST matrix elements behavior is shown. In order to have insight on the scale invariant regime we plot the matrix elements as a function of the normalized scale ℓ/L. This allows the comparison of numerical data from clusters of a different size, dropping out the finite size effects due to the lower and upper cutoff of simulations. The figures show the matrix elements in the full range of the ℓ/L values. The scale invariant regime is in the

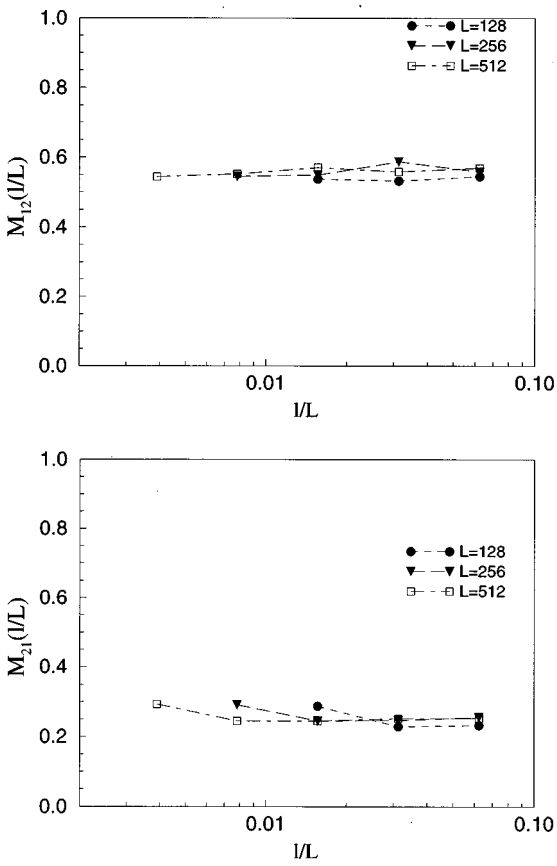

FIG. 2. Behavior of the matrix elements $\mathcal{M}_{1,2}(\ell/L)$ and $\mathcal{M}_{2,1}(\ell/L)$ vs the ''normalized'' rescaling length ℓ/L, for different sizes $L=128,256,512$ of the system. A scale invariant regime appears over an order of magnitude of ℓ/L values.

region $1/L\ll\ell/L\ll1$ [13]. We therefore consider only values of ℓ/L which are at least an order of magnitude inside the above window.

For the smaller simulation ($L=128$) the scale invariant regime is not well defined except for a few points. For the largest size ($L=512$) we have a significant plateau over an order of magnitude or more. This plateau identifies the scale invariant regime for the FST matrix elements. It is worthwhile to remark that, independently of the size of the simulation, the matrix elements have a very good collapse on the same numerical values. In addition, if a larger cluster size is used, the matrix elements behavior is more stable. An extrapolation of $\mathcal{M}_{1,2}$ and $\mathcal{M}_{2,1}$ in the scale invariant regime gives the following values: $\mathcal{M}_{1,2}\simeq0.55\pm0.01$ and $\mathcal{M}_{2,1}\simeq0.25\pm0.01$. By using these numerical values in Eq.(2) to estimate the fractal dimension of DLA, we get $D_f\simeq1.75$, in good agreement with the numerical value $D_f\simeq1.65$ obtained with a box-counting procedure [10]. The results can also be improved by using a refined version of the method such as more complicated coarse-graining procedures or larger cluster realizations. In fact, finite size effects, as well as unavoidable approximations introduced in the box covering algorithm, could affect the MCFST results.

It is interesting to compare the MCFST results with the analytical FST values [1,14]. The MCFST method gives a convolution of the FST matrix elements for the various possible boundary conditions. So, we have to consider the FST

analytical results obtained in the open-closed boundary conditions approximation. The expression for the $M_{i,j}$ in the open-closed approximation is [14]

$$M_{i,j}=M_{i,j}^{op}(1-P_0)+M_{i,j}^{cl}P_0, \tag{3}$$

where $M_{i,j}^{op}$ and $M_{i,j}^{cl}$ are the FST matrix elements, respectively, in open and closed boundary conditions and P_0 is the probability to have closed boundary conditions. In this case, the analytical values of $M_{1,2}$ and of $M_{2,1}$ are in a range of 10–15 % from the numerical values. In particular our MC estimation for $\mathcal{M}_{2,1}$ is quite lower than the analytical result. However, the analytical results are only approximated ones. In order to get the ''exact'' values of the matrix elements one should consider the whole path integral series for the matrix elements and to implement the FST analytical computation for all the possible boundary conditions. This would lead to a lower value of $M_{2,1}$ and to a greater value of $M_{1,2}$, reducing the discrepancy with numerical values. Nevertheless, the comparison of MCFST with the analytical FST tells us that even the crude open-closed approximations is a reasonable analytical truncation which gives very good results.

In summary, we have presented a Monte Carlo procedure which evaluates explicitly the FST matrix elements, allowing the computation of scaling exponents. For the DLA model we have shown the actual implementation of the MCFST scheme. The behavior of the matrix elements has been studied and a scale invariant regime is found. In this regime the results obtained are in good agreement with the analytical ones and previous numerical results. This scheme overcomes the problems arising in the analytical evaluation of the scale invariant dynamics, and is particularly useful for the study of models with long range interactions. The MCFST seems to be a general method and a good alternative calculation scheme that can be easily extended to other models with nonlocal dynamics, like invasion percolation [15] and the quenched dielectric breakdown model [16].

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