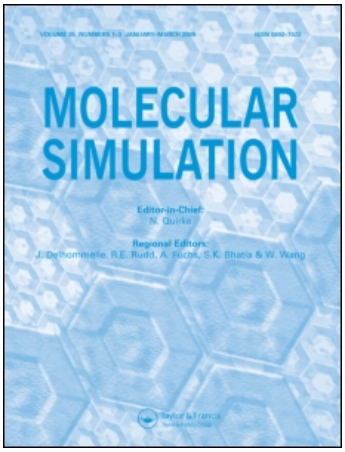

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IFS-SIMULATION OF TRANSPORT PHENOMENA ON COMPLEX FRACTAL MEDIA

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We present in this work an off-lattice method of simulating transport phenomena on fractal structures based on the properties of Iterated Function Systems. The main advantages of this method, compared to classical lattice simulations are the facility of simulating transport processes on a great variety of fractal structures, the possibility of an accurate control of the lengthscale-approximation and the capability of simulating easily complex field-effects on the motion of diffusive particles. Some computer simulation data on fractal structures obtained with this method are presented.

KEY WORDS: Transport phenomena, complex media, fractals, iterated function systems.

INTRODUCTION

One of the main applications of fractal concepts in physical sciences is related to the analysis of transport phenomena and Brownian motion. When the structure of the medium on which the particles diffuse is complex (e.g. percolation clusters at the criticality, fractal media etc.) the geometrical constraints of the medium hinder the motion of the particles and the propagation of the diffusion front is slowed down. This diffusional regime is called anomalous diffusion [1–2]. The propagation of the diffusion front can be estimated from the mean square displacement $\langle \Delta x^2(t) \rangle$ of the particles. In unbiased anomalous diffusion, i.e. when a particle has equal probability of going in next time into one of the nearest neighbouring sites of its actual position, the mean square displacement scales as:

$$\langle \Delta x^2(t) \rangle \sim t^{\beta} \tag{1}$$

when β is less than one (regular Gaussian diffusion gives $\beta = 1$) and equal to the ratio of the fractal dimension D and the fracton dimension D_s of the medium [3]. The anomalous features of transport phenomena on complex media are strongly related to the statistical self-similarity (fractality) of the medium.

Exact theoretical results for transport phenomena on complex structure are very scanty. Consequently the principal way of approaching these problems is to make use of computer simulations.

In most case the simulation of transport phenomena and of diffusion limited processes in complex fractal media is based on lattice approximation of the structure and often requires great computer power.

We present in this paper an off-lattice method for simulating transport phenomena on fractal media based on the properties of Iterated Function Systems (IFS) [4–5].

This method is strongly related to the intrinsic dynamic definition of fractal sets [6–7]. The IFS-diffusion algorithm allows us to simulate a great variety of transport phenomena under different conditions, on a practically unlimited variety of fractals. Moreover the lengthscale on which the diffusion is observed can be easily controlled. It should be said that the IFS-diffusion algorithm can also be used on small computers. All the simulations presented in this work were obtained with a personal computers.

IFS SIMULATION OF TRANSPORT PHENOMENA

As demonstrated by Barnsley and his coworkers [4–6], IFS provide the simplest way of generating fractal objects. An IFS in $\mathbb{R}^n$ is given by the pair $\{\omega_i, p_i\}$, where $i = 1, \ldots, N$, ω_i are contractive transformations mapping $\mathbb{R}^n$ into itself, and p_i are probability weights normalized to one. Given a compact set $\mathscr{C} \subset \mathbb{R}^n$ and the set of transformation ω_i such that

$$\mathscr{C} = \bigcup_{i=1}^{N} \omega_i(\mathscr{C}) \tag{2}$$

the generation of the set $\mathscr{C}$ via IFS system $\{\omega_i, p_i\}$ is ensured by a general theorem (Random Iteration Theorem) [4]: the dynamical system:

$$x_{n+1} = \omega_i(x_n) \text{ prob. } p_i,\ x_n \in \mathbb{R}^n \tag{3}$$

admits the set $\mathscr{C}$ defined by (2) as the limit set (attractor), independently of the values of the weights p_i, which are all assumed to be different from zero. While the transformations ω_i control the geometrical structure of the limit attractor, the weights p_i are responsible to the structure of the invariant ergodic measure [7] associated to (3). Therefore IFS make it possible to generate asymptotically a limit set $\mathscr{C}$ once given its dynamical code $\{\omega_i, p_i\}$. Condition (2) in the Random Iteration Theorem coincides with the Hutchinson definition of invariant compact set, and ultimately of fractal sets [8].

Starting from this mathematical background, it is possible to transform the generation of a compact set $\mathscr{C}$ into a diffusion dynamics on it [9]. In order to do this let us consider a set of N identical IFS generating the same set $\mathscr{C}$ with the same values of the weights p_i. Let us choose a point x_0 on $\mathscr{C}$ as the initial position of a particle, and a positive number d which can be called the radius of diffusion. The next position of the particle in its random motion on $\mathscr{C}$ can be obtained by choosing at random a point obtained from the N IFS that lies inside the ball $\mathscr{B}(x_0, d)$ centered on x_0. The dynamics of the particle can be obtained by iterating this procedure.

The parameter d makes it possible to control the minimal lengthscale at which the particles "feel" the geometrical details of the structure. More precisely, the mean free path of the particles is porportional to d [9]. When the weights p_i are chosen so that the limit invariant density is uniform, then the IFS-diffusion algorithm generates an unbiased diffusion (purely random motion) on the structure. As an example, the scaling of $\langle \Delta x^2(t) \rangle$ vs. t is shown in Figure 1 for the case of the Sierpinski carpets. Using IFS, this fractal can be generated using eight simplitudes of the same scaling ratio $s = 1/3$. Correspondingly, the unbiased diffusional regime is obtained when the weights are all equal: $p_i = 1/8$. The resulting value for the scaling exponent β obtained from IFS-simulation with $d = 0.01$ is given by $\beta = 0.938$, Figure 1, and is

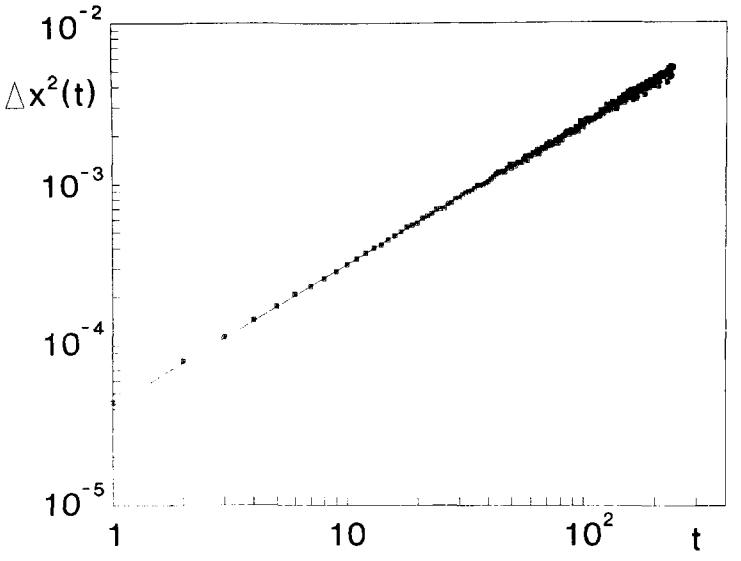

Figure 1 Log-log plot of the mean square displacement vs. time t for unbiased diffusion on Sierpinski carpet, $d = 0.01$.

close agreement with the theoretical results $\beta = 0.9471$ obtained by making use of decimation techniques. Of course, as d decreases the more accurate the simulation of the random walk on the set $\mathscr{C}$ becomes.

From the above discussion it is easy to see that given the IFS-code of a structure, transport phenomena on it can be studied by making use of the IFS-diffusion algorithm, in particular, the IFS-diffusion algorithm can improve our knowledge of the role of fine details of the medium (such as dangling ends, closed loops etc.) on the diffusional propagation.

SIMULATION OF FIELD EFFECTS

In chemical engineering science, the study of transport phenomena in porous media and on percolation beds, and the analysis of mass transport in multicomponent mixtures leads us to consider the case of biased diffusion, i.e. when a mean velocity field (e.g. due to gravity effect in percolation problem) is applied and forces the motion of the particles in one definite direction. In computer simulation terms, a velocity field corresponds to a probability field imposed on the motion of the random walkers. In this section we discuss two important extensions of IFS-simulation in order to cover field-controlled diffusion. In particular, the multifractal random walk is a novel and peculiar feature of IFS-diffusion.

Cartesian biased diffusion

Cartesian biased diffusion corresponds to a constant velocity field directed towards one specific direction. However, despite its simplicity, the theoretical results on this

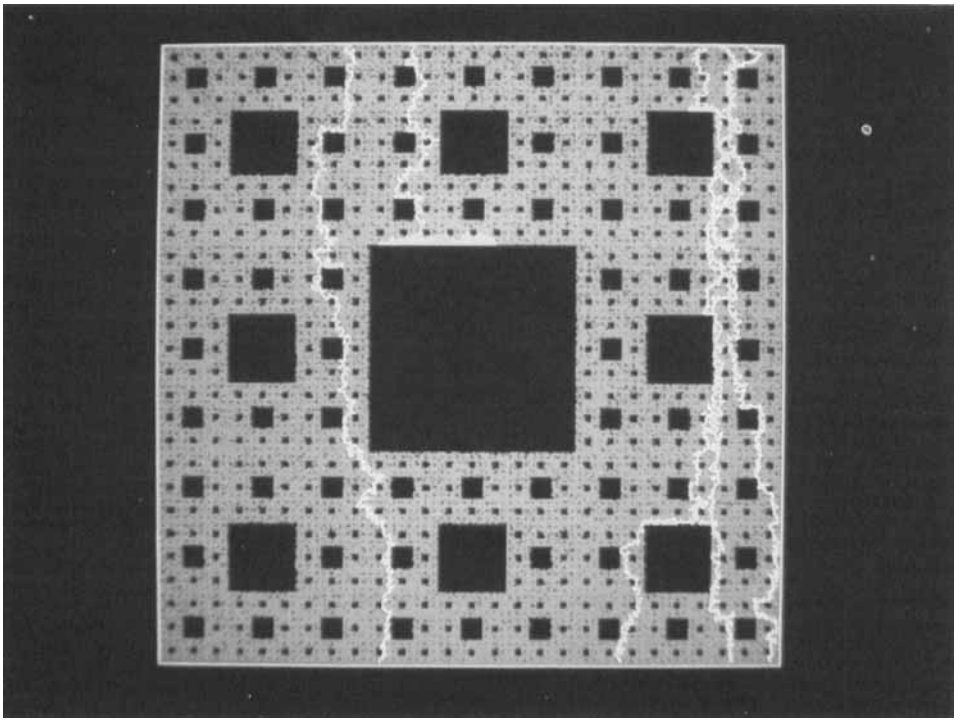

Figure 2 Cartesian biased diffusion of particles on Sierpinski carpet, $d = 0.005$, $p = 0.7$. (See colour plate I).

topic are controversial [2]. The simulation of a Cartesian bias using IFS-diffusion is straightforward. For simplicity, let us consider that in a two-dimensional structure the field is directed from the top to the bottom, and the probability of going down is $p > 1/2$. The constant probability field can be simulated by picking in a selective way a point among those which lie inside the ball $\mathscr{B}(x_n, d)$ of the actual position x_n: we can group them into two sets S_d and S_u representing respectively those points lying below and above x_n and select the next state from S_d with probability p or S_u with probability $(1\text{-}p)$. Figure 2 shows the result of a Cartesian biased diffusion on the Sierpinski carpet with $d = 0.005$, $p = 0.75$. Figure 3 shows the graph of the mean square displacement for $p = 0.7$ and $p = 0.8$., from which obtains asymptotically ($t \gg 1$) for the convective regime:

$$\langle \Delta x^2(t) \rangle \sim \mathscr{H} t^{\gamma} \tag{4}$$

with a value of $\gamma = 1.84 \pm 0.05$. A preliminary study of biased diffusion on both the Sierpinski carpet and the Sierpinski gasket seem to lead to the conclusion that for Cartesian biased diffusion on two dimensional fractal structures the scaling exponent γ is equal to the fractal dimension D (Sierpinski carper has $D = \log 8/\log 3 = 1.893$).

The exponent γ is related to the perimeter scaling of a generic walk around the set of holes of the fractal structures. In the case of the Sierpinski gasket it can be shown that the dimensional exponent related to the perimeter scaling is equal to D [10]. However it must be noted that the Sierpinski carpet can be considered as an *homogeneous fractal* with respect to biased diffusion: independent of the direction of the field

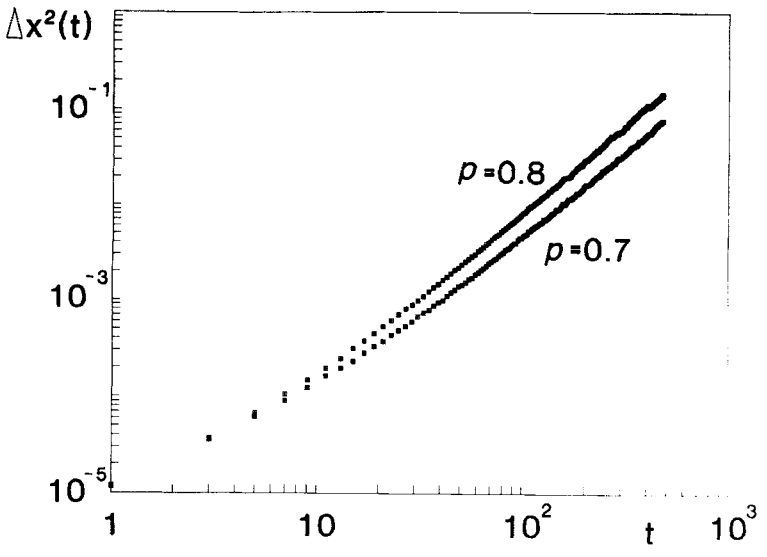

Figure 3 Log-log plot of the mean square displacement vs. time t, $d = 0.005$.

between two generic points there is a path in the direction of the field connecting the two points. The homogeneity of fractals is a consequence of the complete connectivity of this fractal medium. The scaling behavior of biased diffusion on fractal structures which do not fulfill this property and cointain dangling bonds can be different and nonisotropic with respect to the field direction.

Relation (4) can be used to estimate directly from mean square displacement data the effective convective velocity field u of the particles in a fractal medium. If we denote with L a characteristic length of the medium from (4) we obtain the expression for the characteristic convection time t_c:

$$t_c = L^{2/\gamma} \mathscr{H}^{-1/\gamma}$$

from which the convective velocity can be evaluated as $u = L/t_c$. The basic hydrodynamic feature of biased diffusion on fractal structure can therefore be evaluated directly from computer simulation data of the mean square displacement [10].

Multifractal Random Walk

The concept of a *multifractal random walk* is a new theoretical model arising naturally from IFS-diffusion simulation.

Let D be the fractal dimension of the set $\mathscr{C}$ defined by (2). When the weights p_i are chosen so that the invariant measure associated with the dynamical system (3) is equal to the proper Hausdorff D-measure of the set $\mathscr{C}$ [11], the IFS-diffusion algorithm simulates a standard random walk which can be regular ($\beta = 1$) or anomalous ($\beta < 1$) depending on the fractal properties of the structure. In all the other cases the invariant ergodic measure associated with (3) is not homogeneous and exhibits multifractal scaling [11]. Correspondingly, the IFS-diffusion is modified by the scaling of the invariant measure of multifractal random walks on fractal structures show that the mean square displacement still exhibits a power law scaling with time, but the value

of the exponent β is lower than in unbiased diffusion. The main feature of the multifractal random walk is that the fracton dimension D_s becomes a function of the weights p_i. In general, the more singular the invariant measure, the lower the value of D_s and of β. This can be understood by considering that the multifractal scaling in the invariant measure associated with (3) acts as a strongly dishomogeneous bias field (similar to a random field) on the motion of the diffusive particles. Some analogy can be drawn between the multifractal random walk and topological biased diffusion [12]. However, it is to be stressed that the physical meaning of the multifractal random walk is that of a diffusive process in a potential field exhibiting fractal properties. For this reason the study of the multifractal random walk can be connected to analysis of complex relaxation dynamics and can be used for the computer simulation of a hierarchical model of relaxation in complex structures [13].

CONCLUSIONS

The application of IFS to simulation of transport phenomena (IFS-diffusion) represents a significant alternative of simulating different diffusional regimes on fractal structures. In this paper the aspects of IFS-diffusion strictly related to transport phenomena has been developed. However, the application of the IFS-diffusion algorithm can be extended to cover the molecular simulation of chemical reaction kinetics and trapping phenomena on fractal media. The concept of the multifractal random walk, which is a generalization of the standard diffusion peculiar to the formal apparatus of the IFS-diffusion, represents a concrete simulation example of random motion in a hierarchical multiscale potential and can be used to test fractal models of relaxation in complex structures.

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APPENDIX — ITERATED FUNCTION SYSTEMS

Given a compact (closed and limited) set $\mathscr{C}$ in a metric space (say $\mathbb{R}^2$) the fundamental idea in the IFS-construction is to obtain a finite number of contractive transformations ω_i such that the union of the images of $\mathscr{C}$ through the ω_i's coincides with $\mathscr{C}$, eq. (2). In particular, if the set $\mathscr{C}$ is self-similar (e.g. the unit square $[0,1] \times [0,1]$, the Sierpinski carpet), condition (2) is equivalent to covering $\mathscr{C}$ with a number of smaller identical copies of $\mathscr{C}$.

In most of the applications of IFS the ω_1's are chosen *affine*. In the plane ($\mathbb{R}^2$), this means that $\omega_i(x)$ is specified by a 2×2 matrix $\mathbf{A}^{(i)}$ and by a translation vector $\mathbf{b}^{(i)}$: $\omega_i(x) = \mathbf{A}^{(i)}x + \mathbf{b}^{(i)}$, where $x = (x_1, x_2)$ and $\mathbf{b}^{(i)} = (b_1^{(i)}, b_2^{(i)})$. As an example, in the case of Sierpinski carpet (Figure 3), one recognizes that this set can be considered as the union of eight identical copies of itself contracted by a scaling factor of 1/3. Therefore the matrices $\mathbf{A}^{(i)}$ are identical and given by $\mathbf{A}^{(i)} = 1/3\ \mathbf{I}$ ($i = 1..8$), $\mathbf{I}$ being the unit matrix. The translation vectors $\mathbf{b}^{(i)}$ can be obtained by translating the reduced copies in order to cover the set.

One great advantage of IFS is that, given the transformation ω_i, the generation of a given set $\mathscr{C}$ can be performed by a random dynamical system, according to (3), assigning to every ω_i a probability weight $p_i > 0$, because $\mathscr{C}$ represents the limit set of (3), independently of the values of the weights p_i. In other terms, starting from a randomly chosen initial position x_0, after a transient evolution, the trajectories of (3) stabilize on $\mathscr{C}$.

As an example, let us consider the unit interval $\mathscr{C} = [0,1]$ on the line. The simplest IFS generating $\mathscr{C}$ is given by the two transformations $\omega_1(x) = x/2$, $\omega_2(x) = (1 + x)/2$, and thus a formal code for (3) is given by:

```
      X = RANDOM (1)
      DO 1 I = 1,N
          R = RANDOM
          IF R.LT.P THEN X = X/2 ELSE X = (1 + X)/2
    1 CONTINUE
```

where $P = p_1$ and random (1) is a random number generator returning a real number between 0 and 1.

Finally, it should be pointed out that the above one-dimensional case is the dynamic counterpart of Mandelbrot's binomial (mutlifractal) process.