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RANDOM STRUCTURES GENERATION BY LATTICE GAS

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ABSTRACT

Lattice gas models use particles moving and interacting on a graph; developed by physicists to simulate complex flows, they can be used to generate random structures on a physical basis. In this paper, we review some recent developments of these models, with the following main topics: after an introduction of the main rules used in the lattice gas models, namely rules of conservations involved in collisions and boundary conditions, applications to complex flows in random porous media are presented; they offer the possibility to estimate their permeability and the properties of dispersion of fluids as a function of the microgeometry. By addition of aggregation rules, it is possible to generate random aggregates, and to study by simulations processes involving nucleation and growth phenomena in a changing velocity field. Examples based on two phase and multiphase media will be presented. By introduction of forces of attraction or of repulsion between various species, immiscible fluid flows, and phase separations can be simulated. Finally, a promising field concerns the implementation of reaction-diffusion models, where in addition to fluid motion are allowed chemical reaction between species.

Key words: lattice gas, simulations, porous media, multiphase textures

INTRODUCTION

The lattice gas models developed by physicists are a powerful tool for the simulation of complex flows. Starting from simple models with a single specie that we briefly recall, it is easy to perform simulations of flows in random porous media for which some transport properties can be estimated. By addition of marked particles and of aggregation rules, random aggregates (even multiphase) can be generated. Other ways of structure generation are obtained from multiple fluids simulations, or from Reaction-Diffusion models derived from the lattice gas.

LATTICE GAS MODELS

The lattice gas models enable to implement simulations of flows on a microscopic level. Here particles with a unit velocity and mass move on the vertices of a graph. This idea goes back at least to Broadwell (1964), and was recently considerably extended to solve hydrodynamics problems, mainly in the field of turbulence (Hardy et al., 1976;

Frisch et al., 1986-1987). In this section, we give the basic rules of construction and some elementary properties of these models.

Basic Rules: In two dimensions, the FHP model proposed by Frisch, Hasslacher and Pomeau (1986) is built on a hexagonal lattice; a population of particles having seven possible velocities (unit velocity with one of the six possible directions on the lattice, or null velocity) moves on the lattice. At most one particle per velocity is allowed on every point of the lattice, which corresponds to an exclusion principle. Therefore the gas can be described by a multi-component random sets, or by seven binary images (one per velocity). During each time step, every particle moves to its nearest neighbour in the direction of its velocity; this results in a *translation* of the corresponding binary images in the appropriate directions. In addition to the translation of particles, rules of interaction between particles are required, namely *collision rules* for the particles of a gas. These redistribute the velocities with the following constraints: preservation of the total mass and momentum (and consequently of the kinetics energy) at every vertex of the graph. The choice of specific rules enables us to change the viscosity of the fluid for simulations. The process is a sequence of cycles involving the propagation of particles and the redistribution of their velocities. It can be shown (Frisch et al., 1987) that on a macroscopic scale, the velocity map satisfies the Navier Stokes equations, which enables us to simulate hydrodynamics. The great advantage of this model is its simplicity for implementation, even for complex boundary conditions such as those occurring during the evolution of a microstructure; since only binary images are used, there is no round-off errors, and the process can be iterated indefinitely. Three dimensional simulations were made possible by the construction of a specific lattice (Frisch et al., 1987).

Boundary conditions: they imply the behaviour of particles when reaching obstacles: if on a vertex located inside a solid obstacle the collision rule is replaced by a bounce-back condition, the simulated fluid respects the usual no-slip condition (the average velocity being equal to zero on the boundary). On the edges of the field, periodic conditions (particles leaving one side of the field are reintroduced with the same velocity on the opposite side) as well as non periodic conditions (with random injection of particles on the open edges of the field, as made in (Jeulin, 1992)) can be used.

Some indications on the evolution equations: we summarize now the main steps and the main assumptions that are used for the derivation of the Navier Stokes equations from the lattice gas model. Complete derivations are available in (Frisch et al., 1987; Gatignol, 1975; Spohn, 1991). Starting from the basic rules, the evolution equations of each population of particles are Boltzmann equations accounting for the balance of particles involved by the translation and the collision rules. At point x and at the time step $t + \delta t$ we have for the number of particles of type i with the velocity u_i:

$$N_i(t + \delta t, x + \overrightarrow{u}_i) = N_i(t, x) + \Delta_i(N) \tag{1}$$

Eq. 1 can be considered as a finite difference version of Eq. 2 below, obtained for $\delta t \to 0$ and for $a \to 0$, a being the size of the grid:

$$\frac{\partial N_i}{\partial t} + \overrightarrow{u}_i . grad N_i = \Delta_i(N) \tag{2}$$

When only head-on collisions between two particles occur, cross products between the variables N_i and N_j occur. For triple collisions, $N_i N_j N_k$ are present, and so on. Together with the preservation of mass ($\sum_{i=1}^{i=n} N_i = N$) and of momentum ($\sum_{i=1}^{i=n} N_i \overrightarrow{u}_i = N \overrightarrow{u}$),

Eq. 2 leads to the continuity and to the momentum equations, where $\overrightarrow{u}$ is the average velocity:

$$\frac{\partial N}{\partial t} + div(N\overrightarrow{u}) = 0 \tag{3}$$

$$\frac{\partial (N u_\alpha)}{\partial t} + \frac{\partial (\Pi_{\alpha\beta})}{\partial \alpha} = 0 \tag{4}$$

where $\Pi_{\alpha\beta} = \sum_k N_k u_{k\alpha} u_{k\beta}$, $u_{k\alpha}$ being the α component of the velocity $\overrightarrow{u_k}$. The next steps in the calculation uses a Chapman-Enskog expansion of $N_i(t,x)$ as a function of the macroscopic variable $\overrightarrow{u(x,t)}$ and of its gradient, up to the second order. It leads to the Navier Stokes equations for incompressible flows, with transport coefficients depending on the $\Delta_i(N)$ terms (which reflect the collision rules) and on the solutions of the Boltzmann equations 1. These involve a dependence on at least the bivariate distributions of N_i and N_j at point x and time t. Equations for these bivariate distributions involve higher order distributions. To avoid a common regression "ad infinitum", new assumptions must be introduced. Usually is made the Boltzmann's approximation, considering that the variables $N_i(x,t)$ are independent at the order required by the multiple collisions. From this assumption, the $N_i(x,t)$ are solutions of non-linear partial differential equations deduced from Eq. 2. Exact general solutions are known only in particular cases (Gatignol, 1975; Broadwell, 1964). A particular solution in the spatial stationary case for mutually excluding particles, as the binary images used in lattice gas simulations, is given by the Fermi-Dirac distribution, when is added the independence between every $N_i(x,t)$ and $N_j(x',t')$. This approximation is claimed to be valid for the limit case of a low particle density $N(x,t)$. In that case it comes

$$N_i = \frac{1}{1 + \exp\left(h + \overrightarrow{q}.\overrightarrow{u}_i\right)} \tag{5}$$

where the vector $\overrightarrow{q}$ and the constant h are deduced from the mass and momentum conservation equations. When the macroscopic velocity u is close to zero, the Fermi-Dirac distribution degenerates into $N_i = d$, where d is the average density, which is the low velocity equilibrium solution. An expansion of the Fermi-Dirac solution in powers of the macroscopic velocity, together with the Chapman-Enskog expansion, gives an estimation of the fluid transport coefficients. Higher order statistics of the random sets generated by the lattice gas populations (such as for instance their covariances) are unknown, despite some attempts to derive them in a similar but different context (Boghosian and Levermore, 1987), where only upper bounds of covariances could be found. If the binary velocity field is replaced by digital fields and if no exclusion rule is acting, the Fermi-Dirac distribution is replaced by the Maxwell-Boltzmann distribution

$$N_i = \exp\left(-h - \overrightarrow{q}.\overrightarrow{u}_i\right) \tag{6}$$

Instead of working with binary images, some authors developed a model based on the use of local probabilities ($0 \leq N_i \leq 1$) and on the Boltzmann independence assumption in every point x for the collision rule (Mac Namara and Zanetti, 1988; Succi et al., 1989). This model named the LBG (Lattice Boltzmann Gas) has a considerable success, since it provides velocity maps without noise, even for small size systems, contrary to the binary model. However, due to the approximations made in the derivation of the model, there

is no guarantee that probabilities are obtained in each step of the calculation.

APPLICATION TO FLOW IN POROUS MEDIA

Starting from images of porous media made of solid grains that cannot be accessed by the fluid particles, it is possible to simulate flows in porous media and to estimate their transport properties (Rothman, 1988; Jeulin, 1992).
Firstly, by appropriate boundary conditions, or by randomly imposing a drift in the velocity at points of the fluid (which is an input of impulsion to fight against the dissipation due to the zero velocity on the boundaries), it is possible to impose a macroscopic **pressure gradient** to a fluid moving through a porous medium. For a given geometry (as for instance for flows in porous media), since the velocity map solution of the boundary conditions is unknown, we start from independently and uniformly distributed velocities. After some iterations (typically twice the length of the field), the velocity map is stabilized. This approach considering the velocity map is the Euler point of view. When the average velocity is proportional to the pressure gradient, it follows the **Darcy's law** relating the macroscopic flux and the pressure gradient, the proportionality factor being the **tensor of permeability**. Thus it becomes possible to estimate the permeability of a porous medium from lattice gas simulations, using a method that operates at an "undermicroscopic" scale, where basic physical conservation rules are applied. At that scale, no partial differential equation is acting, and the boundary conditions are easily handled. The simulation leaves a population of particles evolve like a dynamic system, until a possible statistical equilibrium is reached. This is a typical simulation of a statistical physics problem. This approach was applied to various Boolean models of porous media, for which were studied the following points (Jeulin, 1992): variability of the permeability induced by the distribution of grains in space; influence of the pore area fraction, of the grain size and of the anisotropy of porous media on the permeability.
Secondly, the **dispersion in porous media** can be studied from the Lagrange point of view: instead of considering the velocity field obtained in the lattice gas simulation, it is possible to **mark** a given particle and to follow its trajectory with time, which builds a random walk (a diffusion process or a Brownian motion with an advective velocity field u). In the present case, the random walk is just the result of the interaction between the marked particles and the other particles in the fluid, respecting the boundary conditions. During the simulation, the velocity of the particle is chosen at random among the possible velocities after each collision. As in (Matheron, 1979), when a macroscopic Fick's law is observed, the coordinates $X_i(t)$ $(i = 1, 2)$ of the trajectory of the marked particle (starting from x (x_i) at time $t = 0$) in the random velocity field $u(x)$ are diffusion stochastic processes with expectation and covariance given by

$$E[X_i(t)] = x_i + \overline{u}_i t \tag{7}$$

$$E[(X_i(t) - x_i - \overline{u}_i t)(X_j(t) - x_j - \overline{u}_j t)] = 2D_{ij}t \tag{8}$$

where $\overline{u}_i$ is the average of the i component of the velocity, while the coefficients D_{ij} build the effective diffusion tensor of an equivalent homogeneous porous medium. The macroscopic coefficients $\overline{u}_i$ and D_{ij} obtained from averages of various particles trajectories are valid for an equivalent homogeneous medium when are fulfilled the conditions for a macroscopic Fick's law to exist; these conditions are unknown in general. For some random media (for instance for self similar, and therefore non stationary porous networks),

Eqs (7,8) are not valid, and a t^{α} (with $\alpha \neq 1$) behaviour is observed (this is called anomalous diffusion). In practice for Boolean porous media simulations, we checked the validity of Eqs (7,8) from the following experimental variograms (with $X_1(t) = X(t)$ and $X_2(t) = Y(t)$), from which a fit to a parabolic curve is looked for:

$$\begin{aligned} 2\gamma_x(\Delta t) &= E[(X(t+\Delta t) - X(t))^2] = 2D_x\Delta t + u_x^2(\Delta t)^2 \\ 2\gamma(\Delta t) &= 2\gamma_x(\Delta t) + 2\gamma_y(\Delta t) = 2(D_x + D_y)\Delta t + (u_x^2 + u_y^2)(\Delta t)^2 \end{aligned} \tag{9}$$

Additional information is obtained from the empirical distribution of the sojourn time τ of the particle in the simulated field, $F_{\tau_a}(t)$. If we consider particles starting from O and leaving the field at the abscissa a at time τ_a, we expect in the case of a constant velocity field (u_x, u_y) and in an infinite homogeneous medium:

$$F_{\tau_a}(t) = P\{\tau_a < t) \tag{10}$$

We have: $X(t) \geq a \Rightarrow \tau_a \leq t$ and therefore

$$P\{X(t) \geq a \mid \tau_a < t\} = \frac{P\{X(t) \geq a\}}{F_{\tau_a}(t)} \tag{11}$$

If $u_x = 0$, by symmetry we have $P\{X(t) \geq a \mid \tau_a < t\} = \dfrac{1}{2}$ and in these conditions

$$F_{\tau_a}(t) = 2P\{X(t) \geq a) \tag{12}$$

When $u_x \gg 0$ and $a > 0$, $P\{X(t) \geq a \mid \tau_a < t\} \simeq 1$ and

$$F_{\tau_a}(t) = P\{X(t) \geq a) \tag{13}$$

In Eqs (12,13) the probability $P\{X(t) \geq a)$ for a Brownian motion with the drift u_x is obtained by

$$P\{X(t) \geq a) = \frac{1}{\sqrt{4\pi D_x t}} \int_a^{+\infty} \exp - \left(\frac{(x - u_x t)^2}{4D_x t} \right) dx \tag{14}$$

The Eqs (12,13,14) were largely used together with Eq. 9 to estimate the diffusive properties of random porous media from simulations (Akulenko, 1995).

Extensions of this approach include three-dimensional flow simulations (Succi et al., 1989; Somers and Rem, 1992), and two-phase flows in porous media (Rothman, 1990). Among the potential domains of application can be mentioned complex flows as encountered in oil reservoirs.

APPLICATION TO SIMULATIONS OF RANDOM MEDIA

Random aggregates: an immediate extension of the lattice gas models is the simulation of **aggregation** (even multiphase) processes (Brémond and Jeulin, 1994). A mixture of a fluid and suspensions is simulated by means of marks (F and S). The standard collision rules are applied on each vertex of the lattice, and the marks are randomly distributed after the collisions. The behaviour of the two types of particles F and S differ during the aggregation process: operating in a field containing obstacles, suspensions are allowed to aggregate (with the probability p^+), and to be bounced back (with the probability $1 - p^+$) when they become the nearest neighbour of an obstacle. Additional conditions

can be introduced for the aggregation, such as: number of aggregated particles in the neighbourhood of a candidate, or directional conditions: the particle may be allowed to aggregate in a neighbourhood made of a cone of 0, 60 or 120 degrees. For instance simulations shown in illustrations were made with the following rules of aggregation: A (0 degree), B (120 degrees), C (120 degrees as for B, and at least 2 of the 3 neighbours must be already aggregated). In addition, particles in the aggregate can leave it for the fluid with the probability p^-, in order to simulate a disintegration process. The growth of an aggregate from a seed at the middle of the field, with a zero average velocity and with the aggregation rule A is illustrated by Fig. 1.

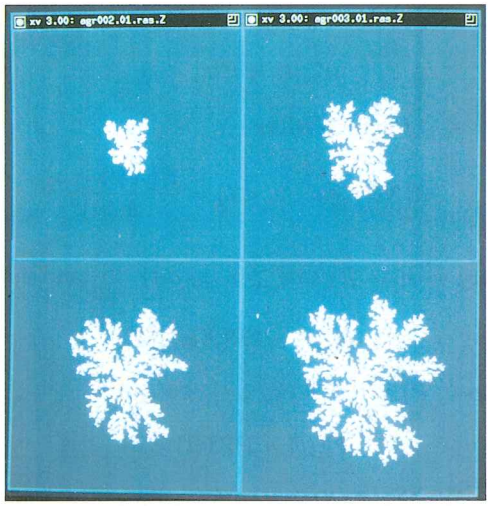

Fig.1. Generation of a random aggregate by rule A: 500, 1000, 1500 and 2000 iterations.

The simulation is made on a 200x200 periodic system. These aggregates are very similar to what is obtained in the so-called DLA (diffusion limited aggregation) model (Witten and Sander, 1981). Addition of a disintegration results into more compact aggregates. Replacing rules A and B by rule C gives less ramified aggregates and quasi dendritic textures as occur in a solidification process are obtained. Interesting morphologies are obtained with non zero velocity on the boundaries of the field: this is illustrated with shear conditions, by forcing the flow in two opposite directions on the upper and the lower boundary as shown in Fig. 2.
The probabilistic properties of these random aggregates, such as $T(K) = P\{K \cap A \neq \emptyset\}$, are not known. Some of them are studied in (Brémond and Jeulin, 1994) from measurements on simulations. It is easy to estimate a "fractal dimension" α from the Eq. 15

$$A(r) = Kr^{\alpha-1}dr \tag{15}$$

where $A(r)$ is the area of the portion of aggregates inside a crown of radius r and of thickness dr, centered on the origin of the aggregate. The parameter α was estimated for each type of aggregation rule, after averaging $A(r)$ over 10 realizations, and keeping $r < 20$. The following results were obtained: $\alpha = 1.736, 1.672$, and 1.813 for rules A, B, C. For comparison, the parameter α obtained for simulations of DLA aggregates built

with random walks of particles on a square lattice is equal to 1.715 (Meakin and Sanders, 1985; Meakin, 1987). This is similar to the results of simulations with the rule A.

Fig. 2. Random aggregate obtained by rule A with shear boundary conditions (5000 iterations).

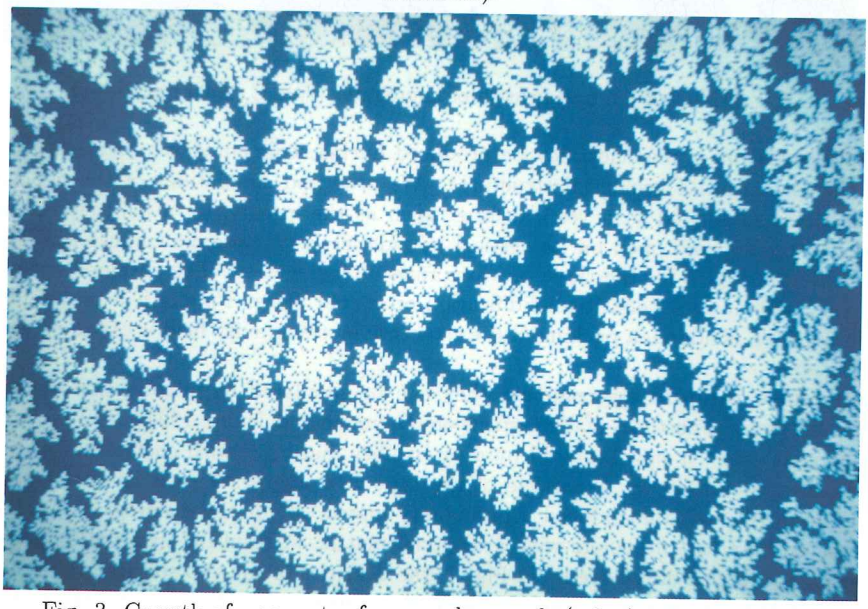

Fig. 3. Growth of aggregates from random seeds (rule A, 2000 iterations)

Another example of aggregation concerns the **nucleation and growth** of a population of aggregates: by replacing the single seed by Poisson points, structures similar to the dendritic solidification out of a melt are obtained; in Fig. 3, an average of 40 seeds per

200x200 image is chosen. There is a competition between the seeds to trap the particles in suspension. In addition, the aggregates are allowed to coalesce. The structure is periodic vertically and horizontally. With a continuous introduction of random seeds, the nucleation generates a dispersion in the sizes of aggregates, as seen on Fig. 4.

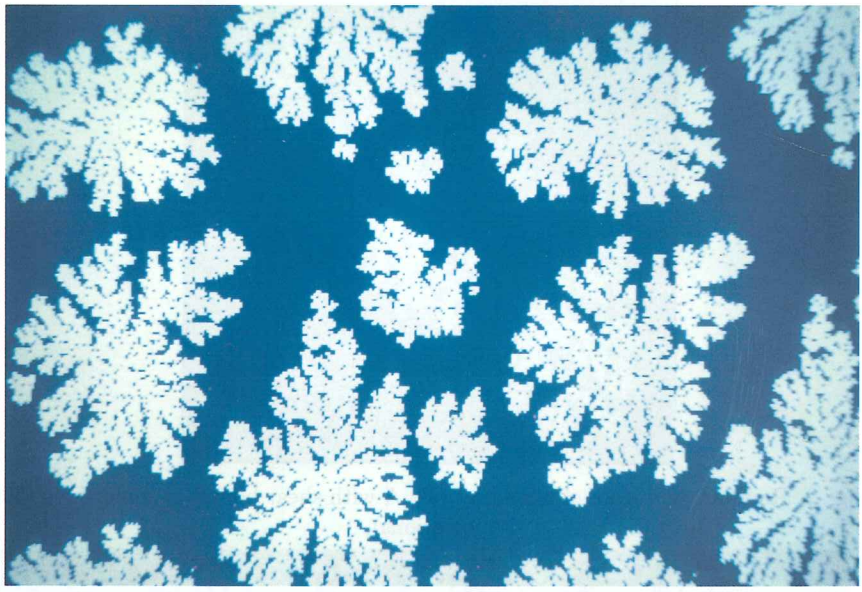

Fig.4. Nucleation and growth of aggregates (rule C, 2000 iterations)

The **deposition** of particles may be produced during sedimentation processes, such as for the formation of geological structures. We produced simulations of the deposition of particles submitted to a vertical force, such as the gravity, on a field closed on its lower boundary, and open on its vertical boundaries, with periodic conditions. This is illustrated in Fig. 5 for the three previous rules of aggregation. The obtained structures are very similar to a dendritic solidification on a cold plate. Finally if a probability of disintegration is added, a packing of the structure by the gravity field is obtained as seen on Fig. 6.

Multiphase random aggregates: they can be simulated by introduction of various colors (A_i) for the particles of the suspension (Brémond and Jeulin, 1994). The probability of aggregation p^+ is now replaced by a probability matrix P with coefficients p_{ij} where p_{ij} is the probability for a particle of the type i to aggregate to a clustered particle A_j. Similarly can be introduced a probability matrix P' for the disintegration. This is illustrated here for two colors with a diagonal matrix P, resulting in a self aggregation process, and with Poisson seeds: in Fig. 7, the densities of the two species are equal and varying, while the density of seeds of specie B is nine times higher than for the specie A. The clusters B can grow normally, while the clusters A are disturbed by clusters B which

produce a wall effect.

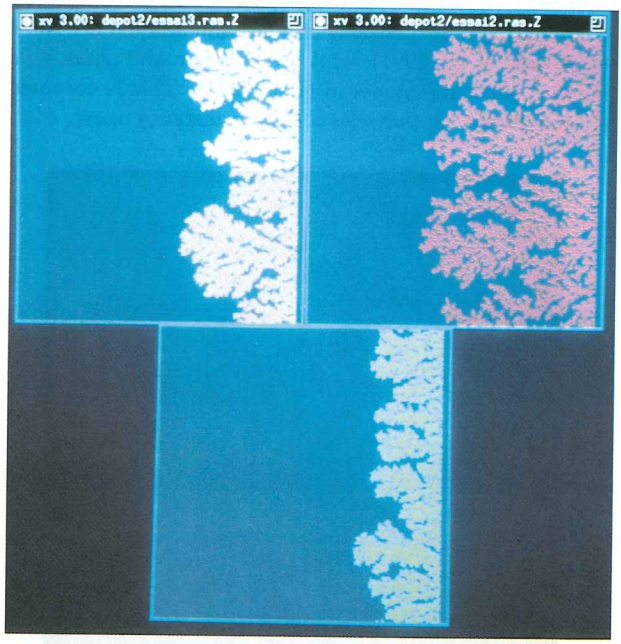

Fig. 5. Deposition of aggregates (rules A, B, C, 5000 iterations)

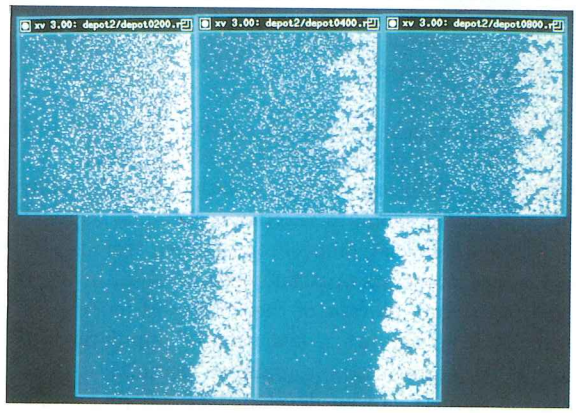

Fig. 6. Deposition and packing of aggregates (rule B after 200, 400, 800, 1600, and 3200 iterations)

Other interesting applications of lattice gas models can be mentioned: flows of suspensions (Ladd et al., 1988); in (Brémond, 1993; Brémond et al., 1995), the filtration of suspensions in liquid iron is simulated, in order to be able to design new filter geometrical properties to optimize the retention of impurities. A model, based on aggregation and disintegration processes, was developed to reproduce the filtration process inside a channel of a ceramic filter. It was calibrated from various experimental data: measurement of the flux of liquid

iron during the filtration; examination of polished sections of clogged filters, where morphological measurements on the obtained aggregates could be compared to the structures generated by the simulations. Suspensions of a gas and a liquid are simulated in (Appert and Zaleski, 1990; Appert et al., 1991), while evaporation and phase separation in porous media are studied with the same model in (Pot, 1994). This is obtained in a clever way by introducing a force attracting particles a certain distance apart.

Fig. 7. Two-phase aggregates (10% red seeds and 90% yellow seeds) in a blue fluid. $p_{ij} = \delta_{ij}$.

REACTION-DIFFUSION MODELS

Finally Reaction-Diffusion models simulating spatial time random structures are studied on lattice gas in (Dab and Boon, 1989; Dab et al., 1990). The potential domains of application of Reaction-Diffusion models is rather broad: study and simulation of microstructures resulting from chemical reactions, chemical segregations during solidification processes; ecological models (competition between various species); biosystems; on a larger scale, geochemical processes or phenomena involved in the environment (dispersion of polluting species...) are relevant of these types of models. In mechanics, certain problems can be modelled in this way: evolution of populations of dislocations, or of microcracks in interaction, segregations in granular media,...

The Reaction-Diffusion models can be developed at different scales: at a macroscopic scale, where the medium is a continuum governed by partial differential equations; at a mesoscopic scale, where all the variables (chemical concentrations, space and time) are discrete; at a microscopic scale where the medium is a set of particles of different species.

Reaction-Diffusion equations: at the macroscopic scale of a continuum, we are looking for the evolution of the chemical concentrations $Z_{jt}(x)$ of the species j $(j = 1, 2, ..., m)$ submitted to chemical reactions and to diffusion. Every component $Z_{jt}(x)$ follows the evolution equation

$$\frac{\partial Z_{jt}(x)}{\partial t} = div(D_j(x) grad Z_{jt}(x)) + F_j(x, t, Z_t) \qquad (16)$$

In Eq. (16), Z_t is the vector with components $Z_{jt}(x)$, $gradZ_{jt}(x)$ is the gradient (with components $\partial Z_{jt}(x)/\partial x_\alpha$) and div is the divergence of a vector field ($div(A) = \sum_\alpha \partial A(x)/\partial x_\alpha$). The variables $Z_{jt}(x)$ are defined in R^n. The $D_j(x)$ are the coefficients of diffusion of the species j. These can be space dependent (diffusion in heterogeneous media) or can be constant. Every $D_j(x)$ is a symmetric, positive definite second order tensor. For an isotropic diffusion in R^n, $D_j(x)$ is a scalar.
The term $F_j(x,t,Z_t)$ is a non linear function of the Z_{jt}. It is usually polynomial, as far as the kinetics of chemical reactions is concerned. For instance, consider the following reaction between four species X_j ($j = 1,2,3,4$)

$$2X_1 + X_2 \rightleftharpoons_{k_2}^{k_1} 2X_3 + X_4 \tag{17}$$

The concentrations Z_{jt} are solutions of Eq. 16 with $F_1(Z_t) = F_2(Z_t) = -k_1 Z_1^2 Z_2 + k_2 Z_3^2 Z_4$ and $F_3(Z_t) = F_4(Z_t) = -F_1(Z_t)$, where k_1 and k_2 are the kinetics constants of the reaction Eq. 17.

Reaction-Diffusion on lattice gas: in (Dab and Boon, 1989; Dab et al., 1990), one specific model (the Schlögl model) was implemented on a square grid. In addition to the collision and translation rules, the chemical reaction term $F_j(x,t,Z_t)$ (a polynomial of degree three in the concentration of a single specie for this model) must be generated. It is obtained on average by means of a birth and death process concerning the number of particles per node, with appropriate transition probabilities. Simulations made in (Dab and Boon, 1989; Dab et al., 1990; Akulenko, 1995) show generation of random structures corresponding to two stable values of the concentration, obtained from local fluctuations of the density of particles.

CONCLUSION

This brief outline of lattice gas models and of their extension intends to demonstrate the potential use of these models for random media generation. Proposed to solve initially complex flow problems, they have a much wider field of applications. Their strength resides in their simplicity of implementation (complex phenomena can be studied from simple rules and with few adjustable parameters). The main difficulties with their use is presently the lack of theoretical results concerning the statistical properties of the generated structures, as opposed to more conventional random sets models. There is undoubtedly work for theory and also for applications in the future.

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