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Random Walkers Cellular Automata for Diffusion Processes

Smooth concentration fields and balance equations for systems of random walkers are obtained by using the coarse-grained space-time averaging method from [5] and averages over the statistical ensemble. This yields a new cellular automaton numerical model for diffusion processes. The number of particles and the averaging space-time scale needed to approximate the concentration, with a given precision, are obtained. Applications were made for systems with small concentrations and diffusion in random fields.

1. Continuous modeling by space-time averages

Let us consider a system of N particles and a *kinematic description* by piece-wise analytic trajectories, $\varphi_i : I \longmapsto \mathbb{R}$, $I = [0,T] \subset \mathbb{R}$, $(1 \leq i \leq N)$. It was proved [6], that the *coarse-grained space-time average* $\langle\varphi\rangle : \mathbb{R}^3 \times (\tau, T-\tau) \longmapsto \mathbb{R}$,

$$\langle\varphi\rangle(\mathbf{r},t) = \frac{1}{2\tau\mathcal{V}} \sum_{i=1}^{N} \int_{t-\tau}^{t+\tau} \varphi_i(t')\, H^+[a^2 - (\mathbf{r}_i(t') - \mathbf{r})^2]\, dt', \tag{1}$$

where $\mathcal{V} = 4\pi a^3/3$ is the volume of the sphere $S(\mathbf{r},a)$ and H^+ the Heaviside left continuous function, has a.e. continuous derivatives in $\mathbb{R}^3 \times (\tau, T-\tau)$ and satisfies the identity

$$\partial_t\langle\varphi\rangle + \partial_\alpha\langle\varphi\xi_\alpha\rangle = \langle d\varphi/dt\rangle. \tag{2}$$

If $\varphi_i(t) = \varphi_i(\eta(t,\omega))$, where $\eta = (\mathbf{r}_1, \cdots, \mathbf{r}_N, \xi_1, \cdots, \xi_N)$ are the trajectories of the stochastic process into the positions-velocities space $\mathbb{R}^{6N}$, we find that the ensemble averages of $\langle\varphi\rangle$, for $a \longrightarrow 0, \tau \longrightarrow 0$, give the usual 'fine-grained' continuous fields of statistical mechanics [3].

Defining the *concentration field* $c(\mathbf{r},t) = \langle 1\rangle(\mathbf{r},t)$ and the *Eulerian velocity field* $u_\alpha(\mathbf{r},t) = \langle\xi_\alpha\rangle(\mathbf{r},t)/c(\mathbf{r},t)$, (1) gives the continuity equation $\partial_t c + \partial_\alpha(cu_\alpha) = 0$. With $cu_\alpha = \langle dx_\alpha/dt\rangle$, defining the *Lagrangian velocity field* $v_\alpha(\mathbf{r},t) = \partial_t\langle x_\alpha\rangle(\mathbf{r},t) + u_\beta\partial_\beta\langle x_\alpha\rangle(\mathbf{r},t)$, and the *diffusion tensor*

$$D_{\alpha\beta}(\mathbf{r},t) = [\langle x_\alpha\rangle(\mathbf{r},t)u_\beta(\mathbf{r},t) - \langle x_\alpha\xi_\beta\rangle(\mathbf{r},t)/c(\mathbf{r},t)], \tag{3}$$

from the continuity equation and (2) we obtain $\partial_t c + \partial_\alpha(cv_\alpha) = \partial_\alpha\partial_\beta(cD_{\alpha\beta})$. Thus, the positivity of coefficients (3) is a test for *diffusive behavior* as described by an advection-diffusion equation.

2. Random walkers cellular automata

Cellular automata describe complex systems by "*fictitious particles* moving in a grid, according to simple and *local rules*, undergoing *simultaneous* changes of states" [2]. We consider N ndependent *random walkers* inside the 1-dimensional grid $\{x_k = k\delta x \mid -m \leq k \leq m\}$. Then the number of particles at the site k is

$$n_k(t+\delta t) = \frac{1}{2}[n_{k-1}(t) + n_{k+1}(t)] - \delta n_{k+1}(t) + \delta n_{k-1}(t), \tag{4}$$

where δn_{k+1} and δn_{k-1} are small for large N. For $n_k(x,t) = c(x,t)\delta x$, (4) becomes the finite-differences diffusion equation, with $D = \delta x^2/2\delta t$, the corresponding diffusion coefficient.

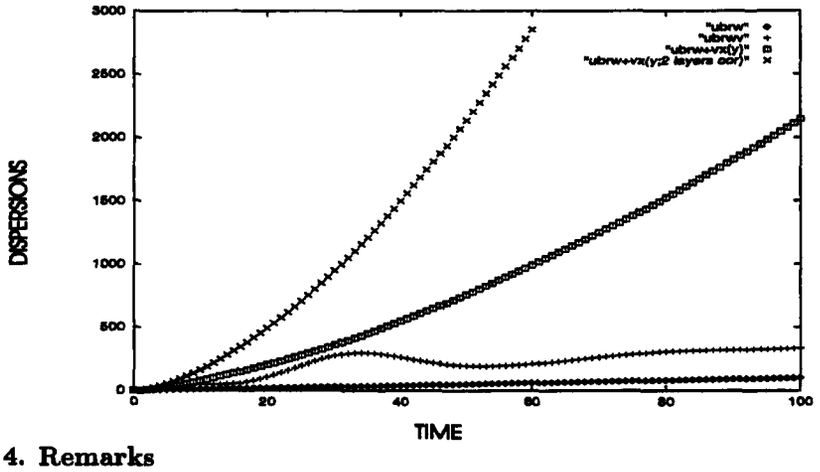
The global estimation, $(\sum_{k=-m}^{m} |n_k - c(x_k,t)\delta x|)/N$, is of order of 10^{-3}, for $N = 10^6$ and $m \geq 30$. Coarse-grained averages (1) over the trajectories of the cellular automaton give the concentration not only in knots but also in any (x,t), reduce the computing time and improve the approximation. By averages over an ensemble of 200 identical cellular automata, it was found that the precision in all the grid is at least 10^{-3}, if a is between $\delta x/8$ and $8\delta x$ and correspondingly, τ is between $10^6\delta t$ and$10^5\delta t$. If the particles reaching the boundaries are instantaneously removed, one finds the mean time needed to eliminate the N particles from the grid to be $\Delta t \sim \ln N$ (i.e. $c \sim e^{-t}$, at small concentrations for systems placed in the previous boundary conditions) [7]. Also, by using a variable step grid, we have verified that there are space-time scales so that (3) gives precise estimations for diffusion coefficients (defined as functions on grid steps by $D = \delta x^2/2\delta t$).

3. Diffusion in random fields

In a similar manner, we built a 2-dimensional random walkers cellular automaton. On it, we superposed an advection given by the samples of a random field and we computed ensemble averages. For horizontal advection and constant velocities in each layer, we get the numerical simulation of the model proposed by Matheron and de Marsily [4],

$$dx^{(\omega_v)}(t) = V(y(t),\omega_v)dt + Ddw(t)\,, \quad dy(t) = Ddw(t)\,,$$

where w is the Wiener process and ω_v labels the realizations of the random field. Diffusive behavior corresponds to $\sigma_x^2(t) \sim t$, where σ_x^2 is the *longitudinal dispersion*, defined by mean square displacements. Using the method from [5] we produced several random advection fields with different correlations. The picture contains dispersions curves given by cellular automaton, for different random advection fields. Unbiased random walk ("ubrw") obviously has a diffusive behavior. For Gaussian ($\sim e^{-y^2}$) correlated longitudinal field we get the nondiffusive behavior reported by Matheron and de Marsily [3], $\sigma_x^2 \sim t^{3/2}$ ("ubrw+vx(y)") and a diffusive long-time behavior, when a constant transversal velocity is added ("ubrwv"). For random fields with identical values in a given number of neighbor layers (the last curve correspond to 2 layesrs correlation), σ_x^2 goes to $\sim t^2$ dependence for increasing correlation length.



4. Remarks

The agreement with 1-dimensional diffusion equation (section 2) and the model of Matheron and de Marsily (section 3) are first proofs of the new numerical model for diffusion processes. These encourage us to use it to study more complex processes, as the challenging problem of transport in heterogeneous porous media. At the same time, we also stress here the possibility to obtain information on the behavior of disordered systems using (3) as a test for diffusive behavior. So, our approach belongs to the attempts to give quantitative definitions of noise and chaos in terms of "divergence between nearby trajectories" [1].

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5. References

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