PERGAMON

Chaos, Solitons and Fractals 11 (2000) 187–192

CHAOS
SOLITONS & FRACTALS

www.elsevier.nl/locate/chaos

A lattice gas automaton approach to "turbulent diffusion"

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Abstract

A periodic Kolmogorov type flow is implemented in a lattice gas automaton. For given aspect ratios of the automaton universe and within a range of Reynolds number values, the averaged flow evolves towards a stationary two-dimensional *ABC* type flow. We show the analogy between the streamlines of the flow in the automaton and the phase plane trajectories of a dynamical system. In practice flows are commonly studied by seeding the fluid with suspended particles which play the role of passive tracers. Since an actual flow is time-dependent and has fluctuations, the tracers exhibit interesting intrinsic dynamics. When tracers are implemented in the automaton and their trajectories are followed, we find that the tracers displacements obey a diffusion law, with "super-diffusion" in the direction orthogonal to the direction of the initial forcing.

1. Introduction

In an incompressible fluid undergoing two-dimensional flow, the equations describing the trajectories of the fluid elements in terms of the stream function ψ take the Hamiltonian form

$$\begin{aligned} \dot{x} &\equiv v_x = -\partial_y \psi(x,y;t), \\ \dot{y} &\equiv v_y = \partial_x \psi(x,y;t), \end{aligned} \tag{1}$$

where $\mathbf{v}$ is the fluid velocity. In practice the trajectories of the fluid elements are visualized by seeding the fluid with suspended particles which act as passive tracers, whose velocity is given by Eq. (1). If the flow were stationary, $\psi_{ss} = \psi(x,y)$, the system would be conservative and thus integrable, and the trajectories of the tracers would coincide with the curves of the contour plot of the stream function. However the actual flow possesses intrinsic fluctuations,

$$\psi(x,y;t) = \psi_{ss}(x,y) + \delta\psi(x,y;t), \tag{2}$$

which in general precludes exact analytical solution of Eq. (1). A consequence of the presence of noise is that the tracers eventually exhibit diffusive behavior. The problem that we address here is the evaluation of the tracer dynamics in the flow (2).

2. Kolmogorov flow

The Navier–Stokes equations for an incompressible fluid subject to an external force $\mathbf{F}$ read

$$\begin{aligned} \partial_t \mathbf{v} + (\mathbf{v}\cdot\nabla)\,\mathbf{v} &= -\rho^{-1}\nabla P + \nu\nabla^2\mathbf{v} + \mathbf{F}, \\ \nabla\cdot\mathbf{v} &= \mathbf{0}, \end{aligned} \tag{3}$$

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PII: S0960-0779(98)00282-3

where P is the hydrostatic pressure, ρ the mass density, and ν the kinematic viscosity. When the flow is two-dimensional and $\mathbf{F}$ has the form

$$\mathbf{F} = \Phi \mathbf{1}_x \cos(\kappa y), \quad \kappa = (2\pi/L), \tag{4}$$

where L is the extension of the system in the y-direction, Eq. (3) describe the periodic Kolmogorov flow [1]. Alternately, with ψ defined by Eq. (1), the Navier–Stokes equations can be recast in the form

$$(\partial_t - \mathrm{Re}^{-1}\nabla^2)\psi + J(\psi, \Delta\psi) = \mathrm{Re}^{-1}\cos(\kappa y), \tag{5}$$

Here $\mathrm{Re} = \psi_0/\nu$ is the Reynolds number, where ψ_0 is defined by $\psi_{\mathrm{ss}} = \psi_0 \cos(\kappa y)$, and $J(\psi, \Delta\psi)$ is the Jacobian

$$J(\psi, \Delta\psi) = \partial_x\psi\partial_y\Delta\psi - \partial_y\psi\partial_x\Delta\psi. \tag{6}$$

By linear stability analysis, one can show that there exists a critical value of the Reynolds number where the system becomes unstable. This is most easily seen by considering a perturbation to the velocity field

$$v_x = v_x^{\mathrm{ss}} + \delta v_x, \quad v_y = v_y^{ss} + \delta v_y \tag{7}$$

with

$$v_x^{\mathrm{ss}} = \frac{\Phi}{\nu\kappa^2}\cos(\kappa y), \quad v_y^{\mathrm{ss}} = 0 \tag{8}$$

and evaluating the perturbation evolution in response to the imposed forcing. We write the perturbation in terms of its spatial Fourier components as

$$\delta v_x(x, y; t) = \mathrm{e}^{\imath qx}\phi(y; t), \quad \delta v_y(x, y; t) = \mathrm{e}^{\imath qx}\varphi(y; t) \tag{9}$$

with

$$\phi(y; t) = \sum_{k=-\infty}^{\infty} \mathrm{e}^{\imath ky}\phi_k(t), \quad \varphi(y; t) = \sum_{k=-\infty}^{\infty} \mathrm{e}^{\imath ky}\varphi_k(t). \tag{10}$$

We insert (7) with (9) and (10) into the Navier–Stokes equations which are then Laplace–Fourier transformed to obtain the characteristic equation and the dispersion equation; retaining only the modes $k = 0, k = \kappa$, and $k = -\kappa$ (i.e. setting to zero the amplitudes of the modes with $|k| > \kappa$), we obtain from the characteristic equation the value of the critical Reynolds number

$$\mathrm{Re}_c = \sqrt{2}\,\nu\kappa^2 \frac{\kappa^2 + q^2}{(\kappa^2 - q^2)^{1/2}}, \tag{11}$$

and from the dispersion equation the modes

$$\delta v_x(q, t) \sim \mathrm{e}^{s_+ t}, \quad s_+ = -\nu\kappa^2 + \nu q^2\epsilon, \tag{12}$$

$$\delta v_y(q, t) \sim \mathrm{e}^{s_- t}, \quad s_- = -\nu q^2\epsilon, \tag{13}$$

with $\epsilon = 1 - (\mathrm{Re}/\mathrm{Re}_c)^2$. Eq. (13) shows that the mode δv_y orthogonal to the direction of the forcing (along the x-axis) exhibits *critical slowing down*, i.e. $s_- \to 0$ when $\mathrm{Re} \to \mathrm{Re}_c$. At $\mathrm{Re} = \mathrm{Re}_c$, the Kolmogorov flow becomes unstable, and beyond the bifurcation ($\mathrm{Re} > \mathrm{Re}_c$) goes into a two-dimensional *ABC* type flow [2] with closed streamlines, separatrices, and infinite trajectories between separatrices, as illustrated in Fig. 1.

3. Lattice gas automaton dynamics

The flow to be investigated is produced by a *lattice gas automaton* [1] which we briefly describe. A lattice gas automaton can be viewed as a collection of particles residing in a discrete space, a regular d-dimensional

[1] For a review on lattice gas automata, see [3].

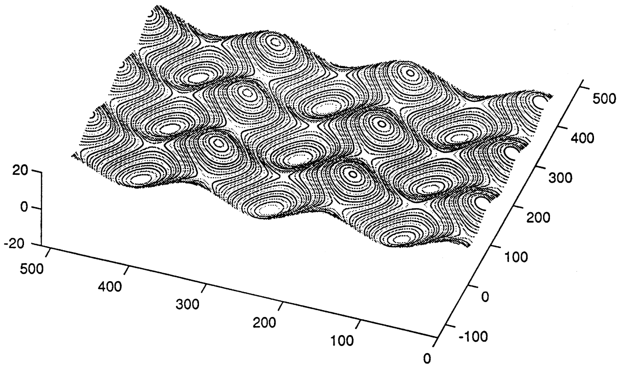


Fig. 1. Contour plot of the stream function $\psi(x,y)$ at $\mathrm{Re}/\mathrm{Re}_c = 2.5$. The streamlines shown here are obtained from the lattice gas automaton described in Section 3 and subject to a periodic forcing according to Eq. (8). The horizontal plane is the $\mathscr{L}$-plane (dimensions are given in lattice units) and the vertical axis gives the amplitude of the stream function $\psi(x,y)$ (in arbitrary units).

lattice $\mathscr{L}$, where they move at discrete time steps. Associated to each lattice node (with position denoted by $\mathbf{r}$) there is a finite set of channels (labeled by Latin indices $i, j, \ldots$). Each of these channels corresponds to a discrete value of the velocity ($\mathbf{c}_i$) that a particle positioned at the specified node may have. An *exclusion principle* imposes that there be a maximum of one particle per channel. The exclusion principle is important because it allows a symbolic representation of the state of the system in terms of bits, and of its dynamics in terms of operations over sets of bits, which are easily implemented on a computer. The state of the automaton at time t is thus described by specifying the *configuration* on each and every node, i.e. the set of bits $\{n_i(\mathbf{r},t)\}_{i=1}^{b}$, $\mathbf{r} \in \mathscr{L}$, for an automaton with b channels per node. The evolution of the automaton takes place in two stages : *propagation* and *collision*, applied sequentially at every time step. Particles are first moved according to their velocity: If channel i at node $\mathbf{r}$ is occupied, the propagation step displaces that particle to channel i of node $\mathbf{r} + \mathbf{c}_i\Delta t$. This updating is done synchronously throughout the lattice. The second stage in the dynamics is a local collision step: As a function of the pre-collisional configuration, a new configuration is chosen by a prescription based on a set of (usually stochastic) rules. This step is crucial to determine the type of physics the automaton will exhibit at the macro- and mesoscopic levels. In particular, the collision step should preserve the quantities that are invariant under the dynamics of the model system. For example, it is possible to construct thermal automata whose rules are such that the number of particles, the momentum and the energy remain unchanged by the collision step [4]. In general, there will be several sets of collision rules consistent with the invariance of the specified constants of motion under the collision step. The choice of a particular set is then dictated by operational convenience, or by the need to explore a particular physical regime. Here we are interested in the two-dimensional hydrodynamic regime and it suffices to implement a simple set of rules governing the automaton dynamics on a triangular lattice [5]. It can be shown, starting from the *microscopic* equations of the automaton, that, provided the symmetry of the lattice is sufficient, the *macroscopic* dynamics of the automaton is consistent with the Navier–Stokes equation [6]. It is one of the virtues of the lattice gas automaton that on the sole basis of microscopic rules in accordance with local invariance and symmetry properties, its macroscopic behavior produces correct hydrodynamics.

Furthermore the lattice gas automaton exhibits two important features: (i) it possesses a large number of degrees of freedom; (ii) its Boolean microscopic nature combined with stochastic micro-dynamics results in *intrinsic spontaneous fluctuations*, and it has been shown that these fluctuations capture the essentials of actual fluctuations in real fluids [7]. Therefore the lattice gas automaton can be considered as a *reservoir of excitations* extending over a wide range of frequencies and wavelengths.

4. Tracer dynamics

Tracers are implemented as suspended particles in the following way. The tracer, which we denote as a t-particle, is subjected to the cooperative effects of the fluid particles, and its dynamics results from the *local* *dynamics* of the automaton, that is from the combined effects of *deterministic* advection (due to the non-zero average velocity field resulting from the constraint imposed to the lattice gas) and *random* advection (due to the automaton intrinsic fluctuations). The t-particle undergoes displacements according to the average velocity of the fluid particles computed over a local domain of $\mathscr{L}$ and over a number (β) of time steps of the automaton ($\beta\Delta t$). In the absence of external force ($\mathrm{Re} = 0$, that is $\psi_0 = 0$ in the notation of Section 2), the dynamics of the t-particle is governed solely by the automaton noise and the tracers undergo random motion leading to diffusive behavior over long distances and long times, i.e. $\langle\delta x^2(t)\rangle = \langle\delta y^2(t)\rangle = 2D_0 t$, for $t \gg \Delta t$, where D_0 will be referred to as the coefficient of *molecular diffusion*, and Δt is the elementary time step of the automaton. The value of β can be varied to modify the effect of noise and thereby to tune the coefficient of molecular diffusion D_0 of the t-particle. So the dynamics of the tracers can be represented in a space defined on a plane parallel to the $\mathscr{L}$-plane and on a time scale set by a time increment equal to $\beta\Delta t$.

We are now interested in the dynamics of the t-particles in a fluid subject to an external force. Therefore we impose a bias to the velocity field of the automaton by preparing its initial state by distributing the velocities of the fluid particles on each node of the lattice so that on the average we obtain a periodic velocity profile according to Eq. (8). With periodic boundary conditions imposed on the automaton universe, the shear triggered by the velocity bias produces a stationary flow in the form of a periodic array of vortices; at a moderately high value of the Reynolds number ($\mathrm{Re}/\mathrm{Re}_c \sim 3$) the spatial structure of the streamlines becomes analogous to the topology of the two-dimensional *ABC* flow. In the absence of noise, the t-particles would follow exactly the streamlines, and their motion would be ballistic. However because intrinsic fluctuations are always present in the automaton (as they are in real fluids), the tracers dynamics can be strongly perturbed, and it is only in the averaged automaton flow that their trajectories reflect the topology of the *ABC* flow, as illustrated in Fig. 2.

When we consider the large-scale, long-time limit ($t \gg L_*/V_*$, where L_* and V_* are the vortex characteristic quantities), we can adopt a Fokker–Planck formulation for the t-particle distribution function $\langle f\rangle$, where the average is taken over the ensemble of realizations and, by averaging over a sufficiently large region of space (*homogenization* hypothesis [8]), we obtain a diffusion-type equation [2]

$$\partial_t\langle\tilde{f}\rangle = D^*_{\alpha\beta}\partial_\alpha\partial_\beta\langle\tilde{f}\rangle, \tag{14}$$

where $\mathbf{D}^* = \mathbf{F}(V_*, L_*, D_0)$ is the *effective diffusion* coefficient of the t-particles in the flow. On the basis of a power law assumption, we infer by dimensional analysis that [3]

$$[D^*] = [D_0]^\mu[L_*]^{1-\mu}[V_*]^{1-\mu}, \tag{15}$$

indicating that for $|\mu| < 1$, and D_0 sufficiently small ($D_0 < L_*V_*$, which is the case in the lattice gas automaton), the elements $D^*_{\alpha\alpha}$ ($D^*_{\alpha\beta} = D^*_{\alpha\alpha}\delta_{\alpha\beta}$) should be larger than D_0, with an important quantitative difference between $D^*_{\alpha\alpha}$ with $\mu > 0$, and $D^*_{\beta\beta}$ with $\mu < 0$.

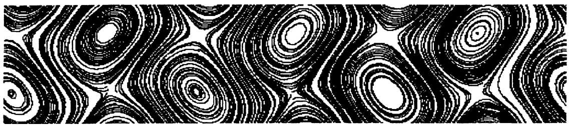
We performed lattice gas automaton simulations as described above, and from measurements of the mean-square displacements of the t-particles $\langle\delta x^2(t)\rangle$ and $\langle\delta y^2(t)\rangle$, we find that over sufficiently long times they exhibit diffusive behavior, as shown in Fig. 3. Notice that in the absence of external force, the mean-square displacement of the t-particle (due to the sole effect of the automaton noise) is isotropic and corresponds to molecular diffusion (full line in Fig. 3).

The diffusion coefficients

$$\begin{aligned} D^*_\parallel &\equiv D_{xx} = \lim_{t\to\infty}\frac{\langle\delta x^2(t)\rangle}{2t}, \\ D^*_\perp &\equiv D_{yy} = \lim_{t\to\infty}\frac{\langle\delta y^2(t)\rangle}{2t} \end{aligned} \tag{16}$$

[2] A complete analysis will be presented elsewhere.

[3] A scaling analysis was also performed by Crisanti et al. in a numerical study of the anisotropic diffusion of a contaminant in the two-dimensional *ABC* flow [9].



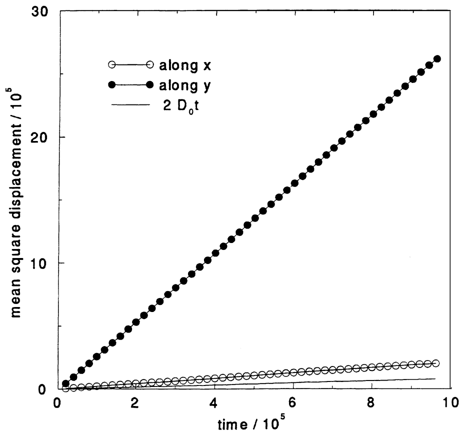


Fig. 2. Tracer trajectories in the flow produced by the automaton with the stream function shown in Fig. 1. The tracer displacements have been averaged over 1000 time steps. Lattice size: 512×128 nodes; average particle density: 0.2 per channel; Reynolds number $\mathrm{Re} = 2.5\mathrm{Re}_c$; Mach number $\mathrm{Ma} < 0.2$.

Fig. 3. Mean-square displacement of tracers measured as a function of time. The data are the projections of the displacements along the x-axis (∘) and y-axis (•), i.e., respectively, along and perpendicular to the direction of the forcing ($\mathbf{F} = F_x(y)\mathbf{1}_x$). The lower full line shows the diffusive behavior generated by the automaton fluctuations in the absence of external force. $\beta = 1$. Distances are given in lattice units and time in automaton time steps.

can be evaluated quantitatively from the explicit expression of the flow and assuming a Gaussian form for the space and time dependence of the second moment of the noise, which is compatible with the spectrum of the automaton fluctuations. We obtain [4]

$$D_\perp^* = \frac{D_0}{1+\chi}, \quad \chi = \frac{\bar{v}_x}{(\langle \delta v_x^2 \rangle)^{1/2}},$$
$$D_\parallel^* = \frac{\bar{v}_x^2}{2\kappa} \frac{1}{D_\perp^*} \frac{1+\frac{1}{2}\chi}{1+\chi^2} + D_\perp^*, \tag{17}$$

where $\langle \delta v_x^2 \rangle$ denotes the automaton fluctuations, and $\bar{v}_x$ the amplitude of the forcing in the velocity field acting on the t-particle: $\dot{x}(t) = \delta v_x(t) + \bar{v}_x \cos(\kappa y)$. In the limit $\bar{v}_x = 0$, one has $D_\perp^* = D_\parallel^* = D_0$, and for $\bar{v}_x \neq 0$, it follows from (17), that $D_\perp^* > D_\parallel^* > D_0$. We find qualitative agreement between these predictions and our simulation data (see Fig. 3).

5. Concluding comments

We have presented an automaton approach to the problem of "turbulent diffusion" in a time-dependent flow with non-trivial average. We have shown the analogy between the stream lines in the averaged flow of the automaton and the phase plane trajectories of the corresponding dynamical system. For the full flow, we obtain agreement between the theoretical value of the diffusion coefficient of the tracers and the corresponding value computed from the lattice gas simulation data. The most important results are: (i) above the critical value of the Reynolds number ($\mathrm{Re} \simeq 3\mathrm{Re}_c$), the tracers dynamics remains diffusive, and (ii) "super-diffusion" is observed in the direction orthogonal to the direction of the forcing ($D_\perp^* \gg D_0$). Higher Reynolds number regimes and flows with non-stationary average are now being investigated.

[4] A complete analysis will be presented elsewhere.

Acknowledgements

JPB acknowledges support by the Fonds National de la Recherche Scientifique (FNRS, Belgium). EVE was supported by the Association Euratom – Etat Belge (Belgium). DH has benefited from a grant from the Fonds pour la Formation à la Recherche dans l'Industrie et l'Agriculture (FRIA, Belgium).

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