Fluctuation-induced first-order transition and dynamic scaling in Rayleigh-Bénard convection

Y. Shiwa, H. Matsunaga, M. Yoshikawa, and H. Yoshitomi
The Physics Laboratories, Kyushu Institute of Technology, Iizuka, Fukuoka 820, Japan
(Received 8 March 1993; revised manuscript received 23 July 1993)

We study the ordering dynamics of the Rayleigh-Bénard convective patterns using the cell-dynamical-system model. Evidence for a fluctuation-induced first-order transition is presented. The simulation result confirms the theoretical prediction to exhibit the dynamic scaling with a characteristic length scale $l(t)\sim t^{1/2}$.

PACS number(s): 47.27.Te, 64.60.Cn, 05.40.+j, 47.20.Ky

When a horizontal layer of fluid is heated from below and driven far from equilibrium, it undergoes a transition, or bifurcation, from a spatially and temporally uniform conducting state to a convecting state of lower symmetry. The structure that emerges above the convective threshold in large aspect-ratio systems is convective rolls of arbitrary orientation. The subsequent evolution of the pattern involves the reorientation of rolls and elimination of defects to attain parallel straight rolls of sizable extent. This Rayleigh-Bénard (RB) convection provides a canonical example of bifurcations and patterns in a nonlinear dissipative system. The phenomena which occur pertain to a broad class of more complex dissipative systems such as liquid crystals and pattern-forming chemical reactions, and have been amenable to highly quantitative studies [1] owing to the relative simplicity of the system. The present paper reports some of the results of a numerical simulation of RB convection for the two-dimensional Langevin model [known as the Swift-Hohenberg (SH) model [2]], using the cell-dynamical-system approach [3,4].

A simplified model of the RB instability was introduced by SH to study the critical behavior associated with fluctuation effects at the bifurcation. It is a two-dimensional theory involving a real order parameter, $\psi(\mathbf{r},t)$, which describes the slow (spatial and temporal) variation of the vertical component of the velocity and the temperature. The variable ψ is also related to the Nusselt number, $\mathcal{N}$, in such a way that $\tilde{\mathcal{N}}\equiv\mathcal{N}-1=S^{-1}\int d\mathbf{r}\,\psi^2(\mathbf{r})$, S being the area of the system. The model is derived from the Oberbeck-Boussinesq equations in the limit of the large Prandtl number, supplemented by the Langevin noise terms. It reads as

$$\begin{aligned}&\tau_0\partial_t\psi(\mathbf{r},t)=-\delta\mathcal{H}\{\psi\}/\delta\psi(\mathbf{r},t)+f(\mathbf{r},t)\ ,\\&\mathcal{H}\{\psi\}=-\int d\mathbf{r}\{(\tfrac{1}{2})\epsilon\psi^2-(\tfrac{1}{4})\tilde{g}\psi^4\\&\qquad\qquad-(\tfrac{1}{2})\tilde{\xi}_0^4[(\nabla^2+q_0^2)\psi]^2\}\ ,\end{aligned}\tag{1}$$

with a Gaussian noise satisfying $\langle f(\mathbf{r},t)f(\mathbf{r}',t')\rangle=2F\tau_0\delta(t-t')\tilde{\xi}_0^2\delta(\mathbf{r}-\mathbf{r}')$. The quantities τ_0, $\tilde{\xi}_0$, q_0, $\tilde{g}$, and F are constants determined for appropriate horizontal boundary conditions [2(b)], and $\epsilon\equiv(R-R_c)/R_c$ is the reduced Rayleigh number with the convective threshold R_c.

An important conclusion of the SH theory is the prediction that because of its high degree of degeneracy of the ordered state the RB convective instability belongs to the Brazovskii universality class [5], where a first-order transition would occur as a result of fluctuations. In ordinary physical systems, however, the strength F of noise (thermal fluctuations) is many orders of magnitude smaller than the typical macroscopic dissipative energies of the system, and the induced fluctuations are extremely weak even for sufficiently small $|\epsilon|$. Since the scale of the predicted jump (say, in $\tilde{\mathcal{N}}$) is set by $F^{2/3}$, it is unobservably small, and in fact the prediction has never been confirmed by the experiments on fluid systems. However, in the numerical simulation it is possible to realize a system with increased effective thermal noise strength. In this manner it is expected that we can make a direct observation of this fluctuation-induced first-order transition. In this connection we note that in symmetric diblock copolymers near the order-disorder transition, which was suspected [6(a)] to be another example of the Brazovskii class, the weak first-order transition has been observed in the laboratory experiment [6(b)]. In that case the fluctuation corrections scale with $N^{-1/3}$, N being the degree of polymerization, and are controllable in practice.

However, it should be pointed out that the perturbation theory of SH breaks down for $L/d\geq F^{-2/5}$ (L and d are the lateral dimension and the plate separation, respectively), and it is not clear how the system will behave in that (strong noise) case. On the other hand, we note that a proper systematic and consistent (e.g., the renormalization-group) theory of the model (1) has still to be worked out. Because of this, a computational study is a valuable source of information.

Motivated by these observations, we have performed simulations of the SH model (1) using the cell-dynamical-system (CDS) approach. The CDS scheme, first proposed by Oono and Puri [3], provides an efficient algorithm for numerical simulations and has proved valuable in studying the late stage of phase-ordering processes such as domain growth in binary alloys. In the CDS scheme the SH equation is replaced by the following equation [4].

$$\begin{aligned}\psi(n,t+1)=&A\tanh\psi(n,t)\\&-L[[\psi(n,t)]_c]_c+B\eta(n,t)\ ,\end{aligned}\tag{2}$$

with $[\psi]_c \equiv \langle\langle \psi \rangle\rangle - c\psi$, where $\psi(n,t)$ is the order parameter in the nth "cell" at time t. The positive constants A, L, c, and B are parameters of our model, B being the noise amplitude; the noise field $\eta(n,t)$ is a random number (uniformly distributed in the interval $[-1,1]$) assigned at each time t to each cell site n. The operator $\langle\langle\ \rangle\rangle$ is the isotropic spatial average, and is defined on the square lattice by $\langle\langle \psi \rangle\rangle = (1/6)\Sigma\psi$ (nearest-neighbor cells) $+(\frac{1}{12})\Sigma\psi$ (next-nearest-neighbor cells). We will refer the reader to Ref. [4] for motivation for replacing the model (1) by the cell dynamics (2).

An important remark is in place in this connection. It is possible to find the following correspondence between the two models by naively applying a conventional Euler algorithm of discretization to equation (1) for small ψ (just above threshold): $A-1 \leftrightarrow \epsilon$, $L \leftrightarrow \tilde{\xi}_0^2/\tau_0$, $c \leftrightarrow q_0^2$, $B^2 \leftrightarrow F$. However, the time increment involved is too large to justify the discretization. The point here is that the CDS model (2) is not the outcome of a simple discretization of the partial differential equation (1). The basic idea of CDS modeling [3] is essentially that of the renormalization-group approach. Namely, if the dynamics of our interest is universal, different physical systems with different equations of motions may be driven to the same fixed point, thereby exhibiting identical asymptotic behavior. Then it is not necessary to solve exactly the equation of motion, if one is interested in the universal behavior. For computational studies one may use a minimal model of the dynamics, which is in the same universality class as the system of interest, but which is computationally more efficient. Conversely, what is observed in the numerical model may be analyzed by a minimal model which is in the same universality class as the model system studied, but which is theoretically more easily handled. We assume that the SH model (1) and the CDS model (2) belong to the same universality class because (i) the local (cell) dynamics is the same in the sense that the relaxational behavior is described by a one-to-one map with two stable and one unstable fixed points; (ii) the interaction among cells is of the type which enhances the stripe patterns above threshold; and (iii) the "up-down" symmetry of the flow (order parameter) field is imposed, so that non-Boussinesq effects are ignored in both models.

In our numerical investigation we have studied a system on a square lattice of size 100×100 with periodic boundary conditions and with parameters $A=1.0015$, $L=0.8$, $c=0.7$, and $B=0.01$. The initial distribution of the ψ's is specified by a random uniform distribution in the range $[-0.01,0.01]$. To average over the initial conditions, we have found that four samples are sufficient to discern the accurate behavior of the quantities studied, as we shall see below.

Given the computationally efficient model, it should be reminded that to estimate the order of transition in numerical computations is a delicate question [7]. Due to finite-size effects, the discontinuity characteristic of the first-order transition is either removed completely or at least smeared out. A hysteresis occurs not only in the first-order transitions but also in the second-order transitions where the relaxation time diverges due to a critical slowing down. We have, therefore, followed Landau and Binder [8] who suggested that the only possibility to distinguish the first-order from the second-order transitions comes from a kinetic analysis by which metastability will show up as a relaxation occurring in two steps. This is because in the second-order transition the rate of relaxation is monotonic. The result is displayed in Fig. 1, where the double-plateau evolution is clearly seen. Since our parameters are likely to be outside of the range of validity of the weak noise limit [although the precise correspondence in parameters between the two models (1) and (2) is not known, as remarked above], we have no theoretical prediction to compare quantitatively with the behavior in the figure. Also shown in the figure are the actual patterns observed at the plateaus. Since the SH theory could not address the pattern achieved at the metastable state, the observed essentially hexagonal pattern will be of help in further elucidating the nature of the transition. Furthermore, in our numerical simulation with periodic boundary conditions and near threshold, all defects eventually disappear to leave straight parallel

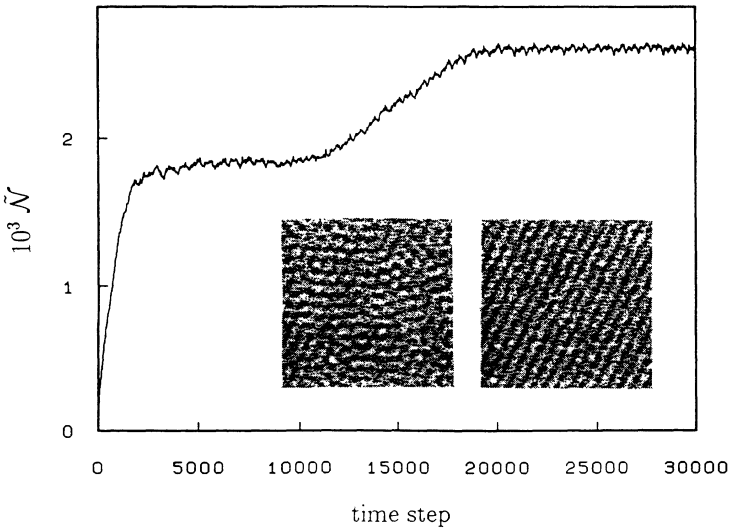

FIG. 1. Time evolution of the Nusselt number $\tilde{N}$ for the stochastic case. Inset: Flow patterns achieved at 7000 and 30 000 time steps; the bright regions show downflow while the dark ones upflow.

rolls asymptotically, in agreement with an earlier observation [9]. The strong constraints imposed by the periodic boundary conditions make all defects anneal out as recognized by Cross [10].

Perhaps against the original motivation of SH, a deterministic version of (1) in which the noise term is omitted is widely used [1] as a model of spatiotemporal pattern formation near the convective threshold. Strangely enough, however, in view of the current intense interest in the study of ordering kinetics [11] from initially unstable states (e.g., the so-called scaling behavior of domain growth in order-disorder transitions), little attention, except the work of Ref. [12], has yet been paid to the comparable study of growth kinetics in RB systems. We have decided to undertake such an investigation. In so doing we should bear in mind the two possible distinctive features of the RB case. First, the interplay with the mode-selection process [1,13]; for $\epsilon>0$ there is a finite band width of modes (wave vectors) of width $\sim\epsilon$ which are stable against small-amplitude perturbations. However, ultimately a well-defined mode seems to be selected as a final stationary state. Second, presence of the critical fluctuations; it is generally believed that the noise effect is unimportant for late-stage ordering kinetics in the ordinary first-order transitions [14]. This is because a zero-temperature fixed point (in the renormalization-group sense) controls the domain growth for all temperatures below a critical temperature [15]. In the case of the noise-induced first-order transition, irrelevance of noise in the growth kinetics is not self-evident. We come back to this later in closing. As a preparatory study towards understanding the complicated interplay of those effects, we consider the deterministic SH model.

In recent work, Elder and Grant [16] have generalized a singular perturbation technique [17,18] (to be referred to as KYG), developed to study the nonconserved ordering kinetics, to a broad class of other ordering dynamics problems of which RB convection is one example. The KYG approach is presumably valid for times long enough that the influence of the initial conditions has decayed, but still short enough that the correlation is not time independent. We will refer to such a time domain as one exhibiting intermediate asymptotics [19]. The extended KYG method formally expands the solution to the deterministic SH equation of (1) in terms of the solution to its linearized part: $\partial_t\psi^0=\gamma(\nabla^2)\psi^0$, where $\gamma(\nabla^2)\equiv\tau_0^{-1}[\epsilon-\tilde{\xi}_0^4(\nabla^2+q_0^2)^2]$. Each term in the expansion is then approximated in the intermediate asymptotics by assuming that $\psi_{\mathbf{q}}^0(t)$, the Fourier transform of $\psi^0(\mathbf{r},t)$, is dominated by its value at $\mathbf{q}=\mathbf{q}_m$; $\mathbf{q}_m$ represents the most unstable mode of the linear dispersion, i.e., $\mathbf{q}_m=\mathbf{q}_0$. Finally the resulting infinite series is resummed to yield $\psi(\mathbf{r},t)=\psi^0(\mathbf{r},t)/\sqrt{(1+\alpha[\psi^0(\mathbf{r},t)]^2)}$, with $\alpha\equiv\tilde{g}/\epsilon$. The quantity of primary interest for our study of evolving order-parameter field is the equal-time correlation function, $g(\mathbf{r}-\mathbf{r}',t)\equiv\langle\psi(\mathbf{r},t)\psi(\mathbf{r}',t)\rangle$. If the initial profile of ψ is spatially uncorrelated and Gaussian distributed, it is straightforward to calculate g at long times. After normalization by $g(0,t)=1$, it is given by $g(\mathbf{r},t)=(2/\pi)\arcsin[\langle\psi^0(\mathbf{r},t)\psi^0(0,t)\rangle/\langle[\psi^0(\mathbf{r},t)]^2\rangle]$. We have calculated the correlator $\langle\psi^0(\mathbf{r},t)\psi^0(0,t)\rangle$ in the manner of KYG [17] to find

$$g(r,t)=(2/\pi)\arcsin\{J_0(q_0r)\exp[-r^2/4l^2(t)]\}\ , \quad (3)$$

where $l(t)=\xi_0\sqrt{2t/\tau_0}$ and $\xi_0\equiv 2q_0\tilde{\xi}_0^2$, with J_0 being the Bessel function of the first kind. With the KYG approach one may take the limit $q_0r\to\infty$, $t\to\infty$ such that r/l remains finite. Hence the result (3) implies the structure factor $S(q,t)$, which is the Fourier transform of $g(r,t)$, has the scaling form $S(q,t)=l^2(t)f[(q-q_0)l(t)]$, apart from the dependence upon q_0 itself; $f(x)$ is a scaling function.

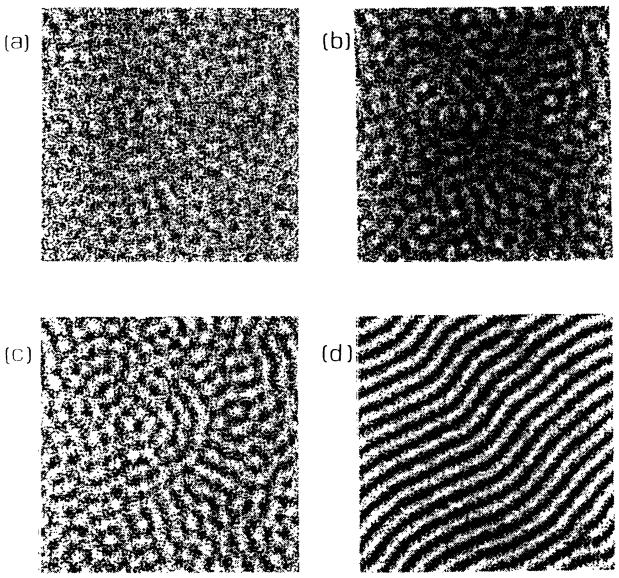

FIG. 2. Flow patterns for the deterministic case at time step: (a) 200, (b) 500, (c) 700, (d) 40 000.

We have used the same CDS scheme (2) as before, but now with $A=1.01$ and $B=0$. Figure 2 exhibits the patterns observed at different times. We computed the circularly averaged (and normalized) correlation function. The length scales $l(t)$ and q_0^{-1} were then calculated by fitting the KYG-like result (3) to the data; $l(t)$ may then be regarded as a measure of the size of domains of uniform rolls. Our results are shown in Figs. 3 and 4. In Fig. 3 we plot the time evolution of $g(r,t)$, where for clarity only the fitted curves are presented [20]. Over the time range shown, the value of q_0 determined from matching could not be distinguished within numerical uncertainty from the value for the most unstable mode of the linear dispersion of (2); $q_m=\arccos[(3c-1)/2]=0.99$ for our system. Our results for $l(t)$ are shown in Fig. 4. The least-squares fit to our data gives an exponent 0.50 ± 0.02, which supports the predicted power-law growth $l(t)\sim t^{1/2}$ in the intermediate asymptotics. At late times a crossover takes place which is not described by the KYG-like solution. Monitoring the heat current $\tilde{\mathcal{N}}$, we observed that the system still continued to evolve. This is probably because the wave number, q_{eq}, of the equilibrium stripe pattern differs from the most unstable mode, q_m, of the linear dispersion, so that the system

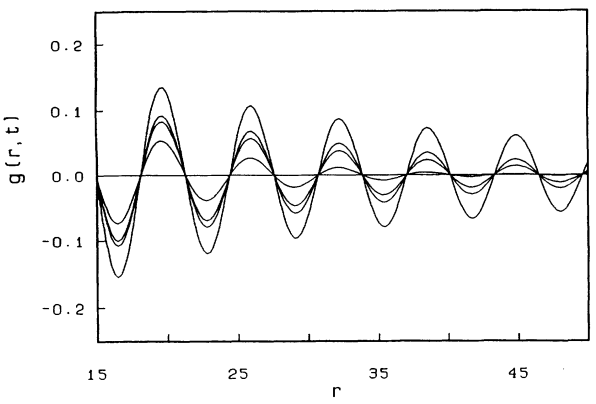

FIG. 3. Correlation function $g(r,t)$ at various times vs distance. The times are the same as in Fig. 2 in order of increasing height.

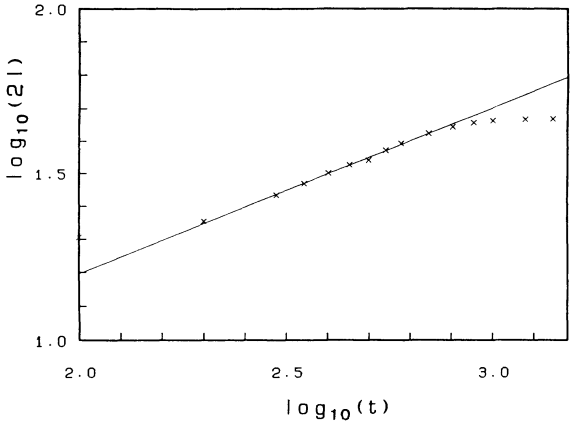

FIG. 4. Plot of our data for $l(t)$ vs time step t. All the data points are obtained by fitting the simulation results to Eq. (3); the standard error of estimates of $l(t)$ is 0.14 at worst. The straight line is the best fit to the data.

tries to attain the length scale $2\pi/q_{eq}$. Such a crossover of the characteristic wave number is absent in the KYG approach. This late-stage phenomena is of interest in connection with the mode selection, and will be the subject of a future study. Finally, we note that Elder, Viñals, and Grant [12] recently carried out the direct simulation of the SH model (1). Comparing the displayed configurations of Ref. [12] with ours, we infer the time regime investigated is te same (intermediate asymptotics) in the two studies. They reported the growth exponent $\frac{1}{5}$ for the deterministic case. We have no explanation to resolve this puzzling discrepancy.

We are presently studying the stochastic CDS model, and preliminary results indicate that (i) the patterns are more ragged than in the deterministic case; (ii) the system evolves with much slower growth rate than the noiseless case. These features are common to phase separation kinetics in the presence of noise [14]. However, in contrast to the latter case, no crossover to the deterministic growth exponent seems to occur. This is compatible with the finding of Elder, Viñals, and Grant [12] who also simulated the stochastic SH model (1) and found the growth exponent $\frac{1}{4}$. The more quantitative aspects of this study will be described elsewhere [21].

In summary, we have reported on numerical studies of the CDS model which we expect to be in the same universality class as the SH model. We observed, for the first time, evidence of fluctuation-induced first-order transition. We also confirmed the theoretical prediction of the generalized KYG approach to SH model to account for the deterministic ordering kinetics at intermediate asymptotics. This, in turn, provides a self-consistency argument for our ansatz that the SH model (1) and the CDS model (2) belong to the same universality class.

Y.S. is grateful to K. Kawasaki and T. Nagai for very helpful comments and discussions.

[1] For recent reviews, see A. C. Newell, in *Lectures in the Sciences of Complexity,* edited by D. Stein (Addison-Wesley, Reading, MA, 1989), p. 107; V. Croquette, Contemp. Phys. **30**, 113, 153 (1989); G. Ahlers, Physica D **51**, 421 (1991); *Pattern Formation in Complex Dissipative Systems,* edited by S. Kai (World Scientific, Singapore, 1992); M. C. Cross and P. C. Hohenberg, Rev. Mod. Phys. **65**, 851 (1993).

[2] (a) J. Swift and P. C. Hohenberg, Phys. Rev. A **15**, 319 (1977); (b) P. C. Hohenberg and J. Swift, *ibid.* **46**, 4773 (1992).

[3] Y. Oono and S. Puri, Phys. Rev. Lett. **58**, 836 (1987); Phys. Rev. A **38**, 434 (1988); S. Puri and Y. Oono, *ibid.* **38**, 1542 (1988). For recent reviews, Y. Oono and A. Shinozaki, Form **4**, 75 (1989).

[4] Y. Oono and Y. Shiwa, Mod. Phys. Let. B **1**, 49 (1987).

[5] S. A. Brazovskii, Zh. Eksp. Teor. Fiz. **68**, 175 (1975) [Sov. Phys. JETP **41**, 85 (1975)].

[6] (a) G. H. Fredrickson and E. Helfand, J. Chem. Phys. **87**, 697 (1987); (b) F. S. Bates, J. H. Rosedale, and G. H. Fredrickson, *ibid.* **92**, 6255 (1990).

[7] For example, see, K. Binder, in *Monte Carlo Methods in Statistical Physics,* edited by K. Binder (Springer-Verlag, Berlin, 1979), p. 1.

[8] D. P. Landau and K. Binder, Phys. Rev. B **17**, 2328 (1978).

[9] H. S. Greenside and W. M. Coughran, Jr., Phys. Rev. A **30**, 398 (1984); however, we remark that this observation was on a deterministic system, and that it was not obvious *a priori* that such a roll state will still be selected in the strong noise case.

[10] M. C. Cross, Phys. Rev. A **25**, 1065 (1982).

[11] For reviews, see, J. D. Gunton, M. San Miguel, and P. S. Sahni, in *Phase Transitions and Critical Phenomena,* edited by C. Domb and J. L. Lebowitz (Academic, London, 1983), Vol. 8; K. Binder, Rep. Prog. Phys. **50**, 783 (1987). For recent developments, see, Ref. 18 and references therein.

[12] K. R. Elder, J. Viñals, and M. Grant, Phys. Rev. Lett. **68**, 3024 (1992); Phys. Rev. A **46**, 7618 (1992).

[13] *Dynamics of Curved Fronts,* edited by P. Pelcé (Academic,

London, 1988).
[14] S. Puri and Y. Oono, J. Phys. A **21**, L15 (1988); Y. Oono, S. Puri, C. Yeung, and M. Bahiana, J. Appl. Crystallogr. **21**, 883 (1988).
[15] Z. W. Lai, G. F. Mazenko, and O. T. Valls, Phys. Rev. B **37**, 9481 (1988); A. J. Bray, *ibid.* **41**, 6724 (1990).
[16] K. R. Elder and M. Grant, J. Phys. A **23**, L803 (1990).
[17] K. Kawasaki, M. C. Yalabik, and J. C. Gunton, Phys. Rev. A **17**, 455 (1978).
[18] K. Kawasaki, Physica A **190**, 161 (1992).
[19] N. Goldenfeld, *Lectures on Phase Transitions and the Renormalization Group* (Addison-Wesley, Reading, MA, 1992).
[20] The data at 40 000 time steps are fitted to the equilibrium correlation function, which can be calculated (Ref. [21]) from Eq. (1) by using an RPA approximation in the absence of noise.
[21] Y. Shiwa (unpublished).

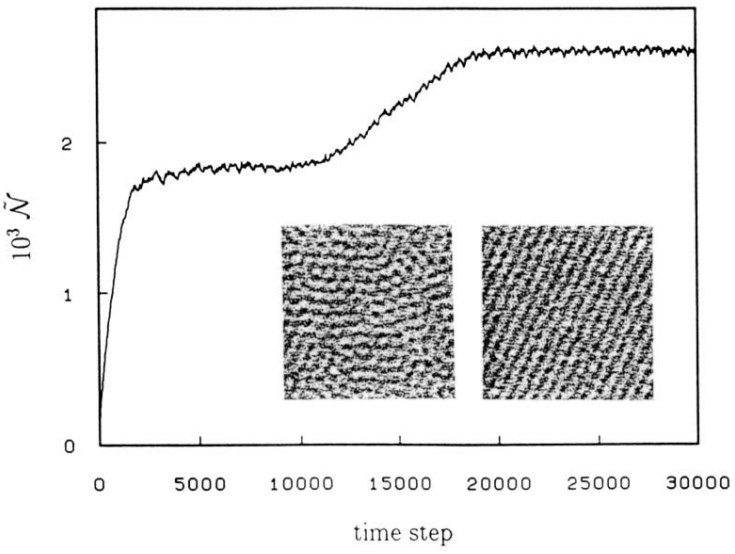

FIG. 1. Time evolution of the Nusselt number $\tilde{N}$ for the stochastic case. Inset: Flow patterns achieved at 7000 and 30 000 time steps; the bright regions show downflow while the dark ones upflow.

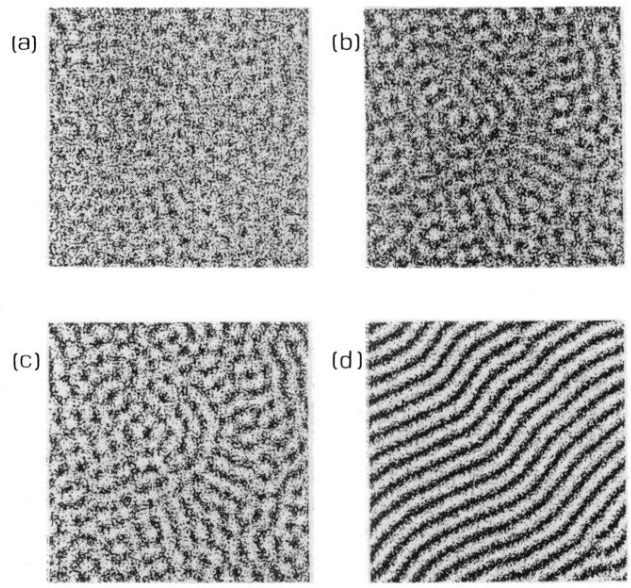

FIG. 2. Flow patterns for the deterministic case at time step: (a) 200, (b) 500, (c) 700, (d) 40 000.