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Bibliography

This bibliography is a compilation of 200 lattice gas references, including theory and computer simulations. References are given in alphabetical order by first author, with the most recent reference first. An attempt was made to include articles published since January 1990 which are related to the article in the April 1986 *Physical Review Letters* by Frisch, Hasslacher, and Pomeau. Some preprints and reports appear also. An electronic file containing an updated form of this bibliography is available upon request from GDD@LANL.GOV.

There are at least two, almost independent, lattice gas communities: one community (whose abstracts appear below) usually moves bits or numbers around a lattice while conserving momentum; the other community, mostly solid-state theorists, focuses almost exclusively on the Ising model. A few of the Ising model papers are included at the end of this bibliography to illustrate areas of interest.

Alexander, F. J., H. Chen, S. Chen, and G. D. Doolen. A lattice-Boltzmann model for compressible fluids, *Physical Review A*, submitted (1992).
The authors formulate a lattice-Boltzmann model which simulates compressible fluids. By choosing the parameters of the equilibrium distribution appropriately, the authors are able to select the sound speed (which may be set arbitrarily low), bulk viscosity and kinematic viscosity. This model simulates compressible flows and can include shocks. With a proper rescaling and with zero sound speed, this model simulates Burgers' equation. The viscosity determined by a Chapman–Enskog expansion compares well with that measured from simulations. The authors also compare the exact solutions of Burgers' equation on the unit circle to solutions of their lattice-Boltzmann model, again finding excellent agreement.

Alexander, F. J., I. Edrei, P. L. Garrido, and J. L. Lebowitz. Phase transitions in a probabilistic cellular automaton: Growth kinetics and critical properties, *J. Stat. Phys.* **68**:497–514 (1992).
We investigate a discrete-time kinetic model without detailed balance which simulates the phase segregation of a quenched binary alloy. The model is a variation on the Rothmann–Keller cellular automaton in which

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particles of type A (B) move toward domains of greater concentration of A (B). Modifications include a fully occupied lattice and the introduction of a temperature-like parameter which endows the system with a stochastic evolution. Using computer simulations, we examine domain growth kinetics in the two-dimensional model. For long times after a quench from disorder, we find that the average domain size $R(t) \sim t^{1/3}$, in agreement with the prediction of Lifshitz–Slyozov–Wagner theory. Using a variety of methods, we analyze the critical properties of the associated second-order transition. Our analysis indicates that this model does not fall within either the Ising or mean-field classes.

Ancona, M. G. Lattice-gas approach to semiconductor device simulation, *Solid-State Electronics* **33**:1633–1642 (1990).
A new approach to semiconductor simulation is presented which is based on a lattice-gas or cellular-automata model and is quite similar to methods recently explored in fluid dynamics. The approach obtains a stochastic solution to the diffusion-drift partial differential equations describing electron transport in semiconductors. The lattice-gas method appears to be fairly well-suited to electron transport simulation with its ability to handle complex geometry, its ease of programming and its stability being some key advantages. In addition, the authors show that the structure of the model itself—its Boolean character—leads to a partial inclusion of electron degeneracy effects. Finally, the authors make a preliminary assessment of the performance of the diffusion-drift lattice-gas model, finding it to be competitive with conventional approaches when its inherent parallelism is fully exploited.

Appert, Cécile, Danile H. Rothman, and Stéphane Zaleski. A liquid–gas model on a lattice, *Physica D* **47**:85–96 (1991).
The authors describe a triangular lattice model able to undergo a liquid–gas transition. The model is obtained by adding an attractive force to the Frisch–Hasslacher–Pomeau gas in the form of non-local interaction. Several types of interactions are suggested and their properties are discussed. When the attractive forces are strong enough the model decomposes into a dense and a light phase. The equation of state of the model is analogous to a van der Waals equation. The theoretical prediction of the equation of state, obtained using a Boltzmann or factorization assumption, agrees well with numerical observations. The isotropy of the model is tested by a numerical computation of the two-dimensional power spectrum.

Appert, Cécile, and Stéphane Zaleski. Lattice gas with a liquid-gas transition, *Phys. Rev. Lett.* **64**:1–4 (1990).
The authors discuss a new momentum-conserving lattice-gas model in

which particles are allowed to exchange momentum between distant sites. The interactions may be tuned so that a first-order transition occurs between a dense and a light phase. An equation of state may be predicted with the assumption that the lattice is in a factorized state just after the particles have propagated. This method accurately predicts the pressure of the stable and unstable states.

Bagnoli, B., F. Chopard, M. Droz, and L. Frachebourg. Critical behavior of a diffusive model with one adsorbing state, *J. Phys. A*, in press (1992).
We study the critical behavior of a nonequilibrium model for adsorption–desorption with diffusion. Without diffusion it is found that the critical exponents belong to the universality class of directed percolation as already shown for sequential dynamics. When diffusion is present, the critical behavior can be described in terms of a crossover between the directed percolation regime and a dynamical mean-field regime associated with the case of arbitrarily large diffusion.

Bardos, C., F. Golse, and D. Levermore. Fluid dynamic limits of discrete velocity kinetic equations, in *Advances in Kinetic Theory and Continuum Mechanics*, R. Gatignol and Soubbaramayer, eds. (Springer-Verlag, Berlin, 1991), pp. 57–71.
The connection between discrete velocity kinetic theory and fluid dynamics is systematically described. Conditions that formally lead to generalized compressible Euler equations or to generalized incompressible Navier–Stokes equations are given. These conditions are related to an H-theorem. A large class of polynomial collision operators in semidetailed balance is proven to satisfy this H-theorem. Finally, results are given concerning the global validity in time of the convergence for the case when the formal scaling leads to the linearized incompressible Navier–Stokes limit.

Bagnoli, F., M. Droz, and L. Frachebourg. Ordering in a one dimensional driven diffuse system with parallel dynamics, *Physica A* **179**:269 (1991).
We study a cellular automata version of a one dimensional lattice-gas model in presence of an external field. This system obeys a generalized Kawasaki like dynamics that conserves the number of particles but privileges particles hopping in one direction. Although the clustering properties do not differ qualitatively from the ones of an equilibrium Ising chain, we observe in our model a sharp transition of the value of the stationary Hamming distance between two randomly chosen configurations submitted to the same thermal noise when varying the temperature or the external field. This transition between a so-called ordered phase and a disordered one reflects the nonequilibrium aspect of the problem.

Benzi, R., and S. Succi. Two-dimensional turbulence with the lattice Boltzmann equation, *J. Phys. A: Math. Gen.* **23**:L1–5 (1990).
The authors investigate the ability of the lattice Boltzmann equation to reproduce the basic physics of fully turbulent two-dimensional flows and present a qualitative estimate of its computational efficiency with respect to other conventional techniques.

Benzi, R., M. Vergassola, and S. Succi. Turbulence modeling by non-hydrodynamic variables, *Europhys. Lett.* **13**(8):727 (1990).

Bernardin, D., O. E. Sero-Guillaume, and C. H. Sun. Multispecies 2D lattice gas with energy levels: Diffusive properties, *Physica D* **47**:169–188 (1991).
The authors consider two particular applications of a multispecies, multi-speed lattice gas with energy levels. In the first one, the authors study the mass diffusion properties of a model where the collisions preserved the partial masses. In the second one, the authors are looking at heat diffusion for a model where the total mass, momentum and energy are the only conserved quantities. The diffusion equations are derived by the Chapman–Enskog method and some numerical simulations are presented.

Bernardin, D., O. E. Sero-Guillaume, and C. H. Sun. Thermal conduction in 2D lattice gases, in *Proceedings Euromech Colloquium 267. Series on Advanced Mathematics for Applied Sciences*, A. S. Alves, ed. (World Scientific, Singapore, 1991), pp. 72–84.
The authors show that for all usual 2D hexagonal models, the only conserved quantities being the total mass, the total momentum and the total energy, one can define a temperature as a function of the density and the internal energy, in such a way that for low mean velocities the heat flux exactly obeys a Fourier law. This expression for the heat flux is derived from the Boltzmann equations using a Chapman–Enskog method. In order to illustrate this property, the authors propose numerical simulations of heat diffusion experiments.

Bernardin, D., and O. E. Sero-Guillaume. Lattice gases mixtures models for mass diffusion, *Eur. J. Mech. B Fluids* **9**(1):21–46 (1990).
A general model for mixtures of gases on a lattice is proposed. Its dissipative properties are studied using a Chapman–Enskog expansion of its Boltzmann Equation. For nonreactive gases, general expressions for the diffusion coefficients and the viscosity are given at low mean velocity. Two-component mixtures are more completely studied and a detailed example is proposed.

Binder, P. M., and M. H. Ernst. Lattice gas automata with time-dependent collision rules, *Physica A* **164**:91–104 (1990).
Particle-scatterer models with time-dependent collision rules in two-dimen-

sional square and triangular lattices are studied. Very good agreement is seen between analytical and molecular dynamics results for the diffusion coefficient at all scatterer concentrations. The results differ significantly from the corresponding analysis for stochastic dynamics. In all square-lattice Lorentz models there is a spurious diffusion mode; its transport coefficient has the same value as the usual diffusion coefficient. The long-time tails with a high frequency modulation, observed in computer simulations, are explained in terms of this spurious mode.

Binder, P. M., and D. Frenkel. Direct measurement of correlation functions in a lattice Lorentz gas, *Phys. Rev. A* **42**:2463 (1990).
We report simulation of a two-dimensional ballistic Lorentz gas on a lattice. A moment-propagation technique allows direct measurements of the velocity correlation function and its moments with low relative errors for all times. We observe the predicted t^{-2} algebraic tails in the velocity correlation function at all studied scatterer densities, unlike what has been reported for continuous systems. In the square lattice, a fast $[(-1)^t]$ oscillation is observed, consistent with the existence of staggered density modes. For the second-rank tensor correlation function we find an extremely slow approach to the expected t^{-3} tail.

Boghosian, Bruce M. Lattice gases illustrate the power of cellular automata in physics, *Computers Phys.* **5**(Nov./Dec.):585–590 (1991).
Over the past few years, lattice-gas simulations have developed into a powerful tool for the study of hydrodynamics and kinetic theory.

Boon, J. P. Statistical mechanics and hydrodynamics of lattice gas automata: An overview, *Physica D* **47**:3–8 (1991).
Some of the issues raised by recent work on lattice gas automata are reviewed.

Boon, J. P., and D. Dab. A class of lattice gas automata for Ginzburg–Landau type equations, in *Proceedings Euromech Colloquium 267. Series on Advanced Mathematics for Applied Sciences*, A. S. Alves, ed. (World Scientific, Singapore, 1991), pp. 230–231.
(No abstract)

Boon, Jean Pierre. Lattice gas automata: A new approach to the simulation of complex flows, in *Microscopic Simulations of Complex Flow*, M. Mareschal, ed. (Plenum Press, New York, 1990), pp. 25–46.
(No abstract)

Brieger, Leesa, and Ernesto Bonomi. A stochastic lattice gas for Burgers' equation: A practical study, *J. Stat. Phys.*, to appear (1992).
We continue our investigation of stochastic lattice gases as a (highly

parallel) means of simulating given PDEs, in this case Burgers' equation in one dimension. The lattice dynamics consist of stochastic unidirectional particle displacement, and our attention is turned toward the reliability of the model, i.e., its ability to reproduce the unique physical solution of Burgers' equation. Lattice gas results are discussed and compared against finite-difference calculations and exact solutions in examples which include shocks and rarefaction waves.

Brieger, Leesa, and Ernesto Bonomi. A stochastic cellular automaton model of nonlinear diffusion and diffusion with reaction, *J. Comp. Phys.* **94**(2):467–486 (1991).
This article presents a stochastic cellular automaton model of diffusion and diffusion with reaction. The master equations for the model are examined and the authors assess the difference between the implementation in which a single particle at a time moves (asynchronous dynamics) and one implementation in which all particles move simultaneously (synchronous dynamics). Biasing locally each particle's random walk, the authors alter the diffusion coefficients of the system. By choosing appropriately the biasing function, the authors can impose a desired non-linear diffusive behavior in the model. The authors present an application of this model, adapted to include two diffusing species, two static species and a chemical reaction in a prototypical simulation of carbonation in concrete.

Brito, R., and M. H. Ernst. Propagating staggered waves in cellular automata fluids, *J. Phys. A* **24**:3331 (1991).
The majority of lattice gases have, apart from the physical conserved quantities of particle number, momentum and energy, spurious ones, usually staggered in space and time. At the level of linear excitations these staggered modes may be purely diffusive or damped propagating waves. In the 8- and 9-bits model on the square lattice we find a large number of new spurious modes, we derive Green–Kubo relations for the diffusivities and damping constants and calculate them in the Boltzmann approximation.

Brito, R., and M. H. Ernst. Lattice gases in slab geometries, *Phys. Rev. A* **44**:8384 (1991).
Non-mean-field type excess correlations at short times are present in 3-D computer simulations of the VACF, but absent in 1-D, 2-D and 4-D. They are caused by ring collisions in a quasi-3-D slab of size $2 \times L \times L \times L$ in a Face Centered Hypercubic lattice with periodic boundary conditions, which is the only available lattice gas cellular automaton with 3-D isotropic fluid flow. We evaluate this excess correlation. The simulation data agree very well with our exact result.

Brito, R., M. H. Ernst, and T. R. Kirkpatrick. Staggered diffusivities in lattice gas cellular automata, *J. Stat. Phys.* **62**:283–295 (1991).
The majority of LGCAs have spurious conservation laws, the so-called staggered invariants, first discovered by Kadanoff, McNamara, and Zanetti. Consequently there are additional hydrodynamic modes of diffusive type, which modify mode coupling theories and the nonlinear fluid dynamic equations. The diffusivities of these staggered modes are evaluated in the mean field approximation for LGCAs on triangular lattices, starting from the Green–Kubo formulas for the staggered diffusivities.

Brito, R., M. H. Ernst, and T. R. Kirkpatrick. Soft modes in CA-fluids at finite wave numbers, in *Proceedings Euromech Colloquium 267. Series on Advanced Mathematics for Applied Sciences*, A. S. Alves, ed. (World Scientific, Singapore, 1991), pp. 198–207.
(No abstract)

Brosa, U. Direct simulation of a permeable membrane, *J. Phys.* (Paris) (1990).
Cellular automata are used to compute flow through a permeable membrane. Scattering centers constitute the membrane. This is in marked contrast to the approach of classical hydrodynamics which represents a membrane by a boundary condition. With the scattering centers the author obtains different, but more plausible results indicating that simple diffusion is the dominating process in a porous layer. The author has thus a case where cellular automata show superiority over the classical methods of theoretical hydrodynamics.

Bussemaker, H. J., and M. H. Ernst. Biased lattice gases with correlated equilibrium states, *J. Stat. Phys.* **68**:431–456 (1992).
The approach to and structure of the equilibrium state is studied for a 7-bit lattice gas with biased forward and backward transition rates by means of mean field theory and computer simulations. If the rate constants obey the factorizability and the detailed balance conditions, the occupations of different velocity directions are uncorrelated, an H-theorem is valid, and a nonuniversal equilibrium state exists that depends explicitly on the transition rates. In case the above conditions are not satisfied, the H-theorem is no longer valid, and mean field theory also predicts nontrivial velocity correlations in postcollision states. The simulations are mainly concentrated on the time dependence of pre- and postcollision velocity correlations on a single node, and on slowly increasing fluctuations that might indicate metastable behavior.

Cabannes, H. On the initial-value problem in discrete kinetic theory, in *Proceedings Euromech Colloquium 267. Series on Advanced Mathematics for Applied Sciences*, A. S. Alves, ed. (World Scientific, Singapore, 1991), pp. 60–71; and *Eur. J. Mech. B Fluids* **10**:207–224 (1991).
The author proves that for some discrete models of the Boltzmann equation, the initial value problem possesses a global solution in time, even for partially negative initial data.

Cabannes, Henri. Global solution of the discrete Boltzmann equation with multiple collisions, *C. R. Acad. Sci. Paris I* **313**:143–148 (1991).
The case of multiple collisions in the discrete Boltzmann equation is considered. We establish sufficient conditions to be verified by the discrete models of the Boltzmann equation, so that the one-dimensional initial value problem possesses a global solution in time, under the constraint that the initial densities and initial mass are positive and bounded.

Cancelliere, A., C. Chang, E. Foti, D. Rothman, and S. Succi. The permeability of a random medium: Comparison of simulation with theory, *Phys. Fluids A* **2**:2085–2088 (1990).
The authors present the results of numerical simulations of the lattice-Boltzmann equation in three-dimensional porous geometries constructed by the random positioning of penetrable spheres of equal radii. Numerical calculations of the permeability are compared with previously-established rigorous variational upper bounds. The numerical calculations approach the variational bounds from below at low solid fractions and are always within one order of magnitude of the best upper bound at high solid-fractions ranging up to 0.98. At solid fractions less than 0.2 the calculated permeabilities compare well with the predictions of Brinkman's effective-medium theory, whereas at higher solid fractions the authors obtain a good fit with a Kozeny–Carman equation. The computations serve as an instructive example of how the lattice-Boltzmann method, a variant of lattice-gas automata, may be applied to the study of flows in complex geometries.

Cantor, Robert S., and Peter M. McIlroy. Statistical thermodynamics of flexible-chain surfactants in monolayer films, *J. Chem. Phys.* **90**:4431 (1989).
A modified cubic lattice model of chain conformations is incorporated within the general theory developed in the preceding article, and used to predict pressure–area isotherms for monolayers at the interface between water and a hydrophobic "solvent." The statistical weight of each cubic lattice conformation is determined by enumerating all rotational isomeric states, and then performing a Boltzmann sum over the set of RIS conformers best described by that cubic lattice state.

Cercignani, Carlo. EUROMECH 267: Discrete models of fluid dynamics, *Transport Theory Stat. Phys.*, to appear (1991).
This is a conference summary of the EUROMECH 267 meeting held in Coimbra, Portugal, September 1990.

Cercignani, C. The trend to equilibrium in discrete and continuous kinetic theory: A comparison, in *Proceedings Euromech Colloquium 267. Series on Advanced Mathematics for Applied Sciences*, A. S. Alves, ed. (World Scientific, Singapore, 1991), pp. 12–21.
The trend to equilibrium can be completely different for the usual kinetic theory with continuous velocity and discrete velocity models. Here a theorem of trend to equilibrium for continuous velocities is proved and a few cases of absence of trend to a homogeneous equilibrium for kinetic models is discussed.

Chan, C. K., and N. Y. Liang. Critical phenomena in an immiscible lattice-gas cellular automaton, *Europhys. Lett.* **13**:495–500 (1990).
A temperaturelike parameter is added to an immiscible lattice gas through the modification of the collision rule in a Monte Carlo manner. It is found that the lattice gas undergoes a phase transition from miscible to immiscible as the temperature is lowered. Critical phenomena similar to those of a thermal system are observed. The critical exponent β of the coexistence curve is found to be 0.3.

Chauvat, Ph., and R. Gatignol. Macroscopic variables in discrete kinetic theory, in *Proceedings Euromech Colloquium 267. Series on Advanced Mathematics for Applied Sciences*, A. S. Alves, ed. (World Scientific, Singapore, 1991), pp. 1–11.
The aim of this paper is to describe a method allowing the determination of summational invariants in discrete kinetic theory. With the velocity vectors, the authors construct two linear spaces: one over the set of rational numbers and the other over the set of real numbers. The authors prove that, if the authors take into account all the collisions, the possible presence of spurious invariants results from the fact that the dimension of the vectorial space generated by the family of the rational numbers is greater than the dimension of the real number space generated by the same vectors. Moreover, the authors give a physical interpretation to all the invariants.

Chen, Hudong, Shiyi Chen, and W. H. Matthaeus. Recovery of the Navier–Stokes equations using a lattice gas Boltzmann method, Bartol Research Institute preprint (1992).
It is known that the FHP lattice gas automaton model and related models possess some rather unphysical effects. These are, (1) a non-Galilean

invariance caused by a density-dependent coefficient in the convection term; and (2) a velocity-dependent equation of state, In this paper, we show that both of these effects can be eliminated exactly in a lattice Boltzmann equation model.

Chen, H., S. Chen, G. D. Doolen, and W. H. Matthaeus. A brief description of lattice gas models for multiphase flows and magnetohydrodynamics, in *1929 Lectures in Complex Systems*, SFI Studies in the Sciences of Complexity, Lecture Volume II, Erica Jen, ed., (Addison-Wesley, 1990), pp. 389–399.
Lattice gas models for single phase fluids, multiphase fluids, and for magnetohydrodynamic fluids are briefly described.

Chen, W., W. H. Matthaeus, and L. W. Klein. Theory of multicolor lattice gas: A cellular automaton Poisson solver, *J. Computational Phys.* **88**:433–466 (1990).
A class of cellular automata models is considered, consisting of a quiescent hydrodynamic lattice gas with multiple-valued passive labels or "colors." Controlled sources of particle color are introduced on the lattice, as are collisions that change individual particle colors while preserving net color. This lattice gas model is shown to be equivalent, in steady state, to a solution to a Poisson equation, with source function proportional to the rate of color introduction and inversely proportional to the intrinsic color diffusivity. The rigorous proofs of the essential features of the multicolor lattice gas are facilitated by use of an equivalent "subparticle" representation in which the color is represented by underlying two-state "spins." Theorems deduced in this way are valid for arbitrary numbers of allowed color values. For example, it is shown that the color diffusivity depends only on the density, for all models of this type. Some preliminary investigations of the efficiency and accuracy of the method are also discussed. Rates of relaxation to the steady state are estimated and schemes for introducing Dirichlet and Neumann boundary conditions are described. Two simple numerical test cases are presented that verify the theory. These results, most of which easily generalize to three dimensions, suggest that a lattice gas of this type may be a useful tool for solution of the Poisson equation.

Chen, Shiyi, Daniel O. Martinez, W. H. Matthaeus, and Hudong Chen. Magnetohydrodynamics computations with lattice gas automata, *J. Stat. Phys.* **68**:591–610 (1992).
Lattice gas automata have received considerable interest for the last several years and possibly may become a powerful numerical method for solving various partial differential equations and modeling different physical phenomena because of their discrete and parallel nature and the capability

of handling complicated boundaries. In this paper, we present recent studies on the lattice gas model for magnetohydrodynamics. The FHP-type lattice gas model has been extended to include a bidirectional random walk process, which allows well-defined statistical quantities, such as velocity and magnetic field, to be computed from the microscopic particle representation. The model incorporates a new sequential particle collision method to increase the range of useful Reynolds numbers in the model, an improvement that may also be of use in other lattice gas models. In the context of a Chapman–Enskog expansion, the model approximates the incompressible magnetic hydrodynamic equations in the limit of low Mach number and high β. Simulation results presented here demonstrate the validity of the model for several basic problems, including sound wave and Alfvén wave propagation and diffusive Kolmogorov-type flows.

Chen, Shiyi, Zhang Wang, Xiaowen Shan, and Gary D. Doolen. Lattice Boltzmann computational fluid dynamics in three dimensions, *J. Stat. Phys.* **68**:379–400 (1992).

The recent development of the lattice gas method and its extension to the lattice Boltzmann method have provided new computational schemes for fluid dynamics. Both methods are fully parallel and can easily model many different physical problems, including flows with complicated boundary conditions. In this paper, basic principles of a lattice Boltzmann computational method are described and applied to several three-dimensional benchmark problems. In most previous lattice gas and lattice Boltzmann methods, a face-centered-hypercubic lattice in four-dimensional space was used to obtain an isotropic stress tensor. To conserve computer memory, we develop a model which requires 14 moving directions instead of the usual 24 directions. Lattice Boltzmann models describing two-phase fluid flows and magnetohydrodynamics can be developed based on this simpler 14-directional lattice. Comparisons between three-dimensional spectral code results and results using our method are given for simple periodic geometry. An important property of the lattice Boltzmann method is that simulations for flow in simple and complex geometries have the same speed and same efficiency, while all other methods, including the spectral method, are unable to model complicated geometries efficiently.

Chen, Shiyi, Hudong Chen, Gary D. Doolen, Semion Gutman, and Minxu Lee. A lattice gas model for thermohydrodynamics, *J. Stat. Phys.* **62**:1121–1151 (1991).

The lattice gas model is extended to include a temperature variable in order to study thermohydrodynamics, the combination of fluid dynamics and heat transfer. The compressible Navier–Stokes equations are derived using a Chapman–Enskog expansion. Heat conduction and convection

problems are investigated, including Bénard convection. It is shown that the usual rescaling procedure can be avoided by controlling the temperature.

Chen, S., H. Chen, G. D. Doolen, Y. C. Lee, and H. Rose. Lattice gas automata models for nonideal gas fluids, *Physica D* **47**:97–111 (1991).
A lattice gas model with a nonideal gas equation of state is presented. Transitions between the solid and gas phase are described. Computer simulations of applications of this model to shock waves are discussed. Generalization of this model to liquid crystal flow is also outlined.

Chen, Shiyi, Hudong Chen, Daniel Martinez, and W. H. Matthaeus. Lattice Boltzmann model for simulation of magnetohydrodynamics, *Phys. Rev. Lett.* **67**:3776–3779 (1991).
A numerical method, based on a discrete Boltzmann equation, is presented for solving the equations of magnetohydrodynamics (MHD). The algorithm provides advantages similar to the cellular automaton method in that it is local and easily adapted to parallel computing environments. Because of much lower noise levels and less stringent requirements on lattice size, the method appears to be more competitive with traditional solution methods. Examples show that the model accurately reproduces both linear and nonlinear MHD phenomena.

Chen, S., K. Diemer, G. D. Doolen, K. Eggert, C. Fu, S. Gutman, and B. J. Travis. Lattice gas automata for flow through porous media, *Physica D* **47**:72–84 (1991).
Lattice gas hydrodynamic models for flows through porous media in two and three dimensions are described. The computational method easily handles arbitrary boundaries and a large range of Reynolds numbers. Darcy's law is confirmed for Poiseuille flow and for complicated boundary flows. Multiply connected pore structures similar to actual sandstone with fixed fractal dimension and porosity are generated. Permeability as a function of fractal dimension and porosity is calculated and compared with results of other methods and experiments.

Chen, S., G. D. Doolen, K. Eggert, D. Grunau, and E. Y. Loh. Lattice gas simulations of one and two-phase fluid flows using the Connection Machine 2, in *Proceedings Euromech Colloquium 267. Series on Advanced Mathematics for Applied Sciences*, A. S. Alves, ed. (World Scientific, Singapore, 1991), pp. 232–248.
In this paper, the authors report recent lattice gas simulations for single-phase and two-phase flows for two-dimensional problems using the Connection Machine 2. For the single-phase fluid problem, the authors use the standard 7-bit lattice gas model with the maximum collision rules. The

velocity and vorticity field of the Kelvin–Helmholtz instability is studied. It is shown that the lattice gas method preserves the main properties of the flow patterns observed in other numerical simulations. Using colored particles and holes, the lattice gas method is extended to simulate immiscible fluids with adjustable surface tension, using a purely local collision scheme. The locality of this model allows us to implement a very fast and parallel algorithm on the Connection Machine 2. Because this new model correctly describes short-range particle–particle interactions between liquids and also particle–solid interactions between the fluid and the wall, cohesion and wettability can be simulated. Applications of the current model to several physical systems including spinodal decomposition, Rayleigh–Taylor flows, and wettability in two-phase flows through porous media are discussed.

Chen, S., G. D. Doolen, K. Eggert, D. Grunau, and E. Y. Loh. Local lattice-gas model for immiscible fluids, *Phys. Rev. A* **43**:7053–7056 (1991).
The authors present a lattice-gas model for two-dimensional immiscible fluid flow with surface tension that uses strictly local collision rules. Instead of using a local total color flux as Somers and Rem [*Physica D* **47**, 39 (1991)], they use local colored holes to be the memory of particles of the same color. Interactions between walls and fluids are included that produce arbitrary contact angles.

Chen, Shiyi, G. D. Doolen, and W. H. Matthaeus. Lattice gas automata for simple and complex fluids, *J. Stat. Phys.* **64**:1133–1162 (1991).
The authors review some recent applications of lattice gas automata, including flow through porous media, phase transitions, thermohydrodynamics, and magnetohydrodynamics.

Chen, Shiyi, Yaosong Chen, and Gary D. Doolen. Lattice gas simulation of viscous flow in a cavity, *Scientia Sinica A* **33**:1072 (1990).
The lattice gas model is extended to include a temperature variable in order to study thermohydrodynamics, the combination of fluid dynamics and heat transfer. The compressible Navier–Stokes equations are derived using a Chapman–Enskog expansion. Heat conduction and convection problems are investigated, including Bénard convection. It is shown that the usual rescaling procedure can be avoided by controlling the temperature.

Cheng, Z., J. L. Lebowitz, and E. R. Speer. Microscopic shock structure in model particle systems: The Boghosian–Levermore cellular automaton revisited, *Commun. Pure Appl. Math.* **44**:971–979 (1991).
The authors carried out new computer simulations of the Boghosian–Levermore stochastic cellular automaton for the Burgers equation. The existence of an extra "conservation law" in the dynamics—even and odd

lattice sites exchange their contents at every time step—implies that the automaton decomposes into two independent subsystems; the simulations show that the density from each subsystem exhibits a "shock front," which does not broaden with time. The location of the shock in a particular microscopic realization differs from that predicted by the Burgers equation by an amount which depends only on the initial microscopic density of the particle system, that is, fluctuations in the stochastic dynamics do not affect the shock profile on the time scale considered. This is in complete accord with theoretical expectations. The apparent broadening of the shock in the original Boghosian–Levermore simulations is shown to result from averaging the two subsystem densities.

Chopard, Bastien, Michel Droz, and L. Frachebourg. Damage spreading and critical behavior of cellular automata models of nonequilibrium phase transition, in *Proceedings of "Evolution and Complexity," Les Houches, March 1990*, R. Livi *et al.*, eds. (Nova Science Publishers, to appear).
Simple cellular automata models of nonequilibrium phase transitions are studied. These markovian models are characterized by the fact that they have two possible states at each site and one adsorbing phase. One shows that, below the transition point, the Hamming distance is exactly related to the one and two-point nonequilibrium correlation function. The divergence of the Hamming distance at criticality gives a precise determination of the transition point. Furthermore, the study of the order parameter near criticality shows that the critical exponent β is not always compatible with the exponent of directed percolation, in contradistinction to a conjecture of Grassberger.

Chopard, Bastien, S. Cornell, and Michel Droz. On the role of fluctuations for inhomogeneous reaction-diffusion phenomena, *Phys. Rev. A* **44**: 4826–4832 (1991).
Although fluctuations have been known to change dramatically the long-time behavior of homogeneous diffusion-reaction phenomena in dimension $d \leqslant 4$, simulations of reaction fronts in two dimensional $A + B \to C$ inhomogeneous systems have only shown marginal departure from mean-field behavior. We perform cellular automata simulations of the one-dimensional case, and find that the width $W(t)$ of the reaction front behaves as $t^{0.293 \pm 0.005}$ in contrast to mean-field behavior $t^{1/6}$. We develop a scaling theory to obtain inequalities for the exponents in the more general mechanism $nA + mB \to C$. Heuristic arguments about the range of fluctuations imply that the mean-field behavior should be correct in dimensions larger than an upper critical dimension $d_{up} = 2$, irrespective of the values of n and m. This leads us to reinterpret the two-dimensional data obtained previously in terms of a logarithmic correction to mean-field behavior.

Chopard, Bastien, and Michel Droz. Microscopic study of the properties of the reaction front in an $A + B \rightarrow C$ reaction-diffusion process, *Europhys. Lett.* **15**:459–464 (1991).
A cellular automata model of the reaction-diffusion process $A + B \rightarrow C$ studied by Gálfi and Rácz is proposed. Numerical simulations on a two-dimensional system show that the reaction rate obeys a scaling form $R(x, t) = t^{-\beta}F(xt^{-\alpha})$, in the long time regime. The exponent α which characterizes the width of the reaction region is found to be 0.186 ± 0.005, in disagreement with the mean field value of 0.1667 obtained by Gálfi and Rácz. Moreover, the discrepancy between the amplitude of the reaction rate of our automata model and its mean field approximation corroborates the belief that the microscopic fluctuations play a relevant role in this nonequilibrium phenomenon.

Chopard, Bastien, and Michel Droz. Cellular automata model for the diffusion equation, *J. Stat. Phys.* **64**:859–892 (1991).
We consider a new Cellular Automata rule for a synchronous random walk on a two-dimensional square lattice, subject to an exclusion principle. It is found that the macroscopic behavior of our model obeys the Telegraphist's equation with an adjustable diffusion constant. By construction, the dynamics of our model is exactly described by a linear discrete Boltzmann equation which is solved analytically for some boundary conditions. Consequently, the connection between the microscopic and the macroscopic descriptions is obtained exactly and the continuous limit studied rigorously. The typical system size for which a true diffusive behavior is observed may be deduced as a function of the parameters entering into the rule. It is shown that a suitable choice of these parameters allows us to consider quite small systems. In particular, our cellular automata model can simulate the Laplace equation to a precision of the order $(\lambda/L)^6$, where L is the size of the system and λ the lattice spacing. Implementation of this algorithm on special purpose machines leads to the fastest way to simulate diffusion on a lattice.

Chopard, Bastien, H. Herrmann, and T. Vicsek. Structures and growth mechanism of mineral dendrites, *Nature* **353**:409–412 (1991).
We investigate the fractal properties of various mineral dendrites. A lattice reaction-diffusion model is proposed to describe the formation of these dendrites and the experimental results are compared with those obtained from numerical simulations.

Chopard, Bastien. A cellular automata model of large scale moving objects, *J. Phys. A* **23**:1671–1687 (1990).
The author proposes a reversible and local rule that allows large scale

objects called "strings" to move with adjustable speed and energy in a three-dimensional space. The author shows that the motion of these strings is governed by discrete Hamiltonian equations and mediated by one longitudinal and two transverse sound waves that propagate along the string. This rule is a first attempt to model a solid body with a cellular automaton. It also provides interesting possibilities for simulating new physical situations.

Chopard, Bastien, and Michel Droz. Cellular automata model for diffusion processes, in *Proceedings of "Evolution and Complexity," Les Houches, March 1990*, R. Livi *et al.*, eds. (Nova Science Publishers, to appear).
The authors study a cellular automata model for a synchronous random walk of many particles subject to an exclusion principle. A diffusive behavior with an adjustable diffusion constant is obtained. The macroscopic and continuous limits of the model are discussed. Deviations from Fick's law $\partial_t \rho = D \nabla^2 \rho$ are observed for finite size systems and non-hydrodynamical regimes. The telegraphers equation appears to be the natural way of describing our model, as a result of the finite speed of the particles. For a stationary state, it is found that the parameters of the rule can be chosen in order to solve with a very good accuracy the Laplace equation, even for small size systems.

Choquet-Bruhat, Y., and G. Pichon. Plasmas with discrete velocities, in *Proceedings Euromech Colloquium 267. Series on Advanced Mathematics for Applied Sciences*, A. S. Alves, ed. (World Scientific, Singapore, 1991), pp. 85–96.
The authors apply the general scheme for discrete Boltzmann equations on a tangent fiber bundle to obtain the Maxwell–Boltzmann system satisfied by a plasma where the velocities take only a finite number of values. The authors show that the system is not strictly hyperbolic in the sense of Leray–Ohya. The authors consider then the case of a plasma in a given electromagnetic field. The authors construct solutions with electric field equal to zero for the magnetic field of a rotating body.

Cliffe, K. A., R. D. Kingdon, and P. Schofield. Lattice gas simulations of free-boundary flows, *Physica D* **47**:275–280 (1991).
Within a very short time, many spectacular results have been produced to demonstrate the potential of lattice gas hydrodynamics (LGH) to predict the behavior of systems governed by the Navier–Stokes and related equations at low to moderate Reynolds numbers. However, in order for LGH to be accepted as an alternative to conventional computational fluid dynamics (CFD) methods for the modeling of flows of practical importance, it is necessary to demonstrate in some specific cases that LGH has

clear advantages over CFD, either where problems remain intractable to the latter or where LGH could give savings in computational resources.

Cohen, E. G. D. New types of diffusion in lattice gas cellular automata, Lectures presented at the Summer school "Microscopic Simulations of Complex Hydrodynamic Phenomena," Alghero, Sardinia (1991). [To be published by Plenum Press, New York (1992).]
These lectures are concerned with Lorentz lattice gas cellular automata (LLGCA), a subclass of lattice gas cellular automata (LGCA). While in LGCA identical point particles move on a lattice and upon encounter scatter according to certain scattering rules, in LLGCA there are two kinds of point particles: moving particles and fixed, i.e., infinitely heavy, particles or scatterers that function as obstacles for the moving particles in their motion through the (in principle infinite) lattice. The name of Lorentz is used here, because he considered for the first the motion of small, light particles through heavy particles. The lattice distance, time step and speed of the moving particles are taken to be in unity. The moving particles move, independently of each other (i.e., there are no collisions between them) along the bonds of a lattice, colliding only with the fixed scatterers. The scatterers are randomly placed on the lattice sites and in this sense one studies motion in a random medium. If a moving particle arrives at an empty lattice site, where there is no scatterer, it moves in the next (discrete) time step to the nearest neighbor lattice site in the direction of its velocity. If the lattice site is occupied by a scatterer, the collision rules prescribe the position and velocity of the particle after the collision, which takes place instantaneously. Two types of collision rules will be considered here: probabilistic and deterministic. In LLGCA there is no momentum conservation of the particles, only number (and energy). As a consequence, diffusion rather than hydrodynamic flow can be studied. The main question is then: what is the nature of the motion of the particles through the obstacles (scatterers)? Is it diffusion, i.e., can it be described by a diffusion equation with a well-defined diffusion coefficient, D? If so, how does this diffusion coefficient depend on the nature and density of the scatterers and to what extent does it mimic diffusion of point particles through obstacles in continuous space and time?

Cornell, S., R. Dickman, M. Droz, and M. C. Marques. Competing two species directed percolation, *J. Phys. A* **24**:5605 (1991).
We study a three-state probabilistic cellular automata describing an extension of conventional directed percolation (DP) with two species (A and B) using mean-field and Monte Carlo methods. The densities of the two species in the steady-state exhibit phase transitions which are due both to simple percolation and to competition between the species. In $1 + 1$ dimen-

sions, as well as a simple DP transition, there is a line of first-order transitions between pure-A and pure-B phases. The phase diagram in $2+1$ dimensions agrees qualitatively with that obtained from mean-field calculations, with second-order transitions between pure and mixed phases. Preliminary studies suggest that the critical exponents are in the same universality class as (one-species) DP.

Cornille, H., and T. Platkowski. Exact solutions of a hierarchy of mixing speeds models, Saclay preprint SPhT/91-181.
This paper presents several new aspects of discrete kinetic theory (DKT). First we propose a hierarchy of d-dimensional ($d=1, 2, 3$) models with (2^d+3)-velocities and three moduli speeds: 0, 2 and a third one which can be arbitrary. We assume that the particles at rest have an internal energy which, for microscopic collisions, supplies for the loss of the kinetic energy. In a more general way than usual, we allow collisions which mix particles with different speeds. Second, for the $(1+1)$-dimensional restriction of the systems of PDE for these models which have two independent quadratic collision terms, we construct different exact solutions. We study the usual types of exact solutions: periodic solutions and shock wave solutions obtained from the standard linearization of the scalar Riccati equations that we call Riccatian shock waves. Then we find other types of solutions of the coupled-Riccati equations that we call non-Riccatian shock waves and compare them with the previous ones. The main new result is that, between the upstream and the downstream states, these new solutions are not necessarily monotonic. Further, for the shock problem, we solve numerically a two-dimensional dynamical system of ODE with limit values corresponding to the upstream and downstream states. As a by-product of our study, we propose two new linearizations for the Riccati coupled equations with two functions.

Cornille, H. Shock waves for the two speeds $8V_i$, $14V_i$ and $24V_i$ discrete Boltzmann models with temperature, in *Proceedings Euromech Colloquium 267. Series on Advanced Mathematics for Applied Sciences*, A. S. Alves, ed. (World Scientific, Singapore, 1991), pp. 131–143.
For the discrete Boltzmann models in R^{q+1}, $q=1, 2, 3$, with two speeds $\sqrt{q+1}$, 1 or 2, the authors consider the shock waves along an axis for both the square $8v_i$, cubic $14v_i$, and hypercubic $24v_i$ models. They satisfy two classes of q-dependent nonlinear equations and the main difference comes from the projections of the speeds along the axis which are either 1 or 1, 2. First the authors compare the two methods of shock wave solutions: either the Rankine–Hugoniot relations for traveling waves or the similarity solutions. The first method does not always lead to positive cross

sections. Second we study the local entropy and temperature overshoots across the shock.

Cornille, H. Exact $(1+1)$-dimensional solutions to the multispeed discrete Boltzmann models, Nonlinear Dispersive Waves, Central Florida Conference SPhT/91-164, March 11–15 (1991).
We present $(1+1)$-dimensional waves which are exact solutions of a hierarchy of discrete Boltzmann models (discrete velocities and densities) and which exhibit a dispersive behavior. A hierarchy is characterized by the number of independent densities, the number of independent collision terms and their system of $(1+1)$-dimensional partial differential equations. These models include both the plane square eight velocity model and the cubic three-dimensional Cabannes model. They are multispeed discrete Boltzmann models with well-defined temperature. These $(1+1)$-dimensional exact solutions are, up to constants, the sums of two exact compressive shock wave solutions, traveling in opposite directions.

Cornille, H. Exact periodic solutions for a class of multispeed discrete Boltzmann models, Nonlinear Coherent Structures in Physics, Saclay SPhT/91-086 June (1991).
Only for multispeed discrete Boltzmann models can we obtain a well-defined temperature. Recently, different hierarchies of multispeed, multidimensional, $(d>1)$, discrete model have been characterized by their $(1+1)$-dimensional partial differential equation along one axis. Here, for the simplest hierarchy with five independent densities and two speeds which are 1 and either $\sqrt{d}$ or $\sqrt{2}$, we construct $(1+1)$-dimensional periodic solutions. The physical corresponding models are the planar square $8v^i$, $d=2$ model and two three-dimensional $14v_i$, $d=3$ models (one of them being the Cabannes model).

Cornille, Henri. $(1+1)$-Dimensional hierarchies of multispeed discrete Boltzmann model equations, *J. Math. Phys.* (1991).
We study multispeed discrete Boltzmann models in R^d satisfying all conservation laws and leading to well-defined temperatures. The $(1+1)$-dimensional restriction of the system of partial differential equations satisfied by the densities of these models can be classified. One class is characterized, along a chosen coordinate, by the number and location of the independent densities and by the number and physical meaning of the independent collision terms. Each class defines a hierarchy of partial differential equations which depends on the dimension, d, of a particular model in R^d. We obtain different classes associated either with two velocity speeds, 1, $\sqrt{2}$ and 1, $\sqrt{d}$, 2, $\sqrt{2}$, and 2, $\sqrt{d}$ or three velocity speeds 0, 1, $\sqrt{2}$ and 0, 2, $\sqrt{2}$. Each class represents a d-hierarchy of a well-known discrete model. We discuss

the simplest exact solutions which are the similarity shock wave solutions and we compare them with the Rankine–Hugoniot solutions.

Cornille, Henri. Exact solutions for two ten-velocity three-dimensional discrete kinetic models, *C. R. Acad. Sci. Paris II* :743–747 (1991).
Recently Cabannes has obtained two discrete kinetic models for the applications to condensation and evaporation problems and Tiem has found an explicit class of periodic solutions. Here we construct exact solution, both self-similar solutions and periodic solutions sums of two self-self-similar complex conjugate waves which are positive for times, $t \geqslant 0$. For the model with only cubic collision terms, we show that necessarily two different classes of solutions exist.

Cornubert, R., D. d'Humières, and D. Levermore. A Knudsen layer theory for lattice gases, *Physica D* **47**:241–259 (1991).
A Knudsen layer theory is presented for lattice gases with arbitrary boundary conditions. Analytical results are obtained for two special orientations, these exhibit anisotropic Knudsen layers provided suitable conditions are satisfied. However, the standard boundary conditions used in previous simulations are shown to be isotropic, the bulk steady state extending everywhere in the gas. This theory allows a more accurate localization of the obstacle with respect to the lattice nodes. These results are in good agreement with the numerical simulations.

Dab, David. Lattice gas automata: a microscopic approach to reactive systems (in French), Ph.D. dissertation, University of Brussels (1992).

Dab, David, Jean-Pierre Boon, and Yue-Xian Li. Lattice-gas automata for coupled reaction-diffusion equations, *Phys. Rev. Lett.* **66**:2535–2538 (1991).
The authors present a lattice-gas automaton approach to coupled reaction-diffusion equations. This approach provides a microscopic basis for exploring systems which exhibit such interesting features as oscillatory behavior and pattern formation. Two-species systems are analyzed in detail. As an application of the formalism, the authors construct the microscopic dynamics for a system described by the Maginu equations; simulation results show excellent agreement with the phenomenological predictions. Most important is the result showing that they obtain Turing-type structures by a purely microscopic approach.

Dab, David, A. Lawniczak, J. P. Boon, and R. Kapral. Cellular automaton model for reactive systems, *Phys. Rev. Lett.* **64**:2462–2465 (1990).
A method for construction of a variety of probabilistic lattice-gas automata for chemically reacting systems is described. The microscopic reactive dynamics gives rise to a general fourth-order polynomial rate law for the average particle density. The reduction of the microdynamical equations to a discrete or continuous Boltzmann equation is presented. Connection

between the linearized Boltzmann equations and a reaction-diffusion macroscopic equation is discussed. As an example of the general formalism, a set of cellular automata rules that yield the Schlogl phenomenological model is constructed. Simulation results are presented.

d'Humières, D., Y. H. Qian, and P. Lallemand. Finding the linear invariants of lattice gases, in *Computational Physics and Cellular Automata*, A. Pires, D. P. Landau, and H. Herrmann, eds. (World Scientific, Singapore, 1990), pp. 97–115.
Hydrodynamical phenomena can be simulated by discrete lattice gas models obeying cellular automata rules with suitable restrictions on the crystallographic symmetries of the underlying lattice. However, the derivation of the dynamical equations assumes that mass, momentum and eventually energy are the only conserved quantities during the time evolution of the automata. We shall present here an exact method to find all the conserved linear quantities of any given model, a method which is equivalent to finding the null space of a matrix derived from the time evolution of the automaton. Thus, the algorithmic complexity is of order N^3, where N is the number of nodes of the lattice. We shall also give a faster method when the model is invariant under the translation group of the lattice. These results will be applied to several one- and two-dimensional models. Finally, we shall note that this method gives the linear invariants of any cellular automaton.

Diemer, K. L., F. J. Alexander, S. Chen, and G. D. Doolen. A local lattice gas for fluids with adjustable miscibility, Los Alamos National Laboratory preprint (1992).
We introduce a local lattice gas model for binary fluids with an adjustable parameter λ which allows us to control the degree of miscibility. For $\lambda < \lambda_c$ the fluids are immiscible while for $\lambda > \lambda_c$ the fluids are miscible. This model is a variation on the one recently developed by Chen *et al.* In this paper, we present theoretical and numerical studies on the diffusive properties of the lattice gas. We demonstrate the utility of this model as a means of simulating flows in various geometries for binary fluids of arbitrary miscibility.

Doolen, G. D. What can we hope for from lattice gas methods?, in *Lecture Notes in Physics 357: Whither Turbulence? Turbulence at the Crossroads*, J. Lumley, ed. (Springer-Verlag, 1990), pp. 397–409.
Although the idea of using discrete methods for modeling partial differential equations occurred very early, the actual statement that cellular automata techniques can approximate the solutions of hydrodynamic partial differential equations was first presented by Frisch, Hasslacher, and Pomeau. Their description of the derivation, which assumes the validity of

the Boltzmann equation, appeared in the *Physical Review Letters* in April 1986. It is the intent of this article to provide a description of the simplest lattice gas model and to examine the successes and inadequacies of a lattice gas calculation of flow in a two-dimensional channel. Some comments will summarize a recent result of a lattice gas simulation of flow through porous media, a problem which is ideal for the lattice gas method. Finally, some remarks will be focused on the impressive speeds which could be obtained from a dedicated lattice gas computer.

Duarte, J. A. M. S., and U. Brosa. Viscous drag by cellular automata, *J. Stat. Phys.* **59**(2):501–508 (1990).
A simple method to compute the drag coefficient of two-dimensional bodies with arbitrary shapes is presented. The procedure is based on cellular automata as an extreme idealization of the molecular dynamics of a viscous fluid. The authors verify the algorithm by examples and obtain results in quantitative agreement with experiments even when eddies behind obstacles are formed.

Dubrulle, B., and U. Frisch. Eddy viscosity of parity-invariant flow, *Phys. Rev. A* **47**:5355–5364 (1991).
A general formalism is developed to determine eddy viscosities for incompressible flow of arbitrary dimensionality subject to forcing periodic in space and time. The dynamics of weak large-scale perturbations is obtained by a multiscale analysis. The large-scale behavior is found to be formally diffusive (first order in time, second order in space) whenever the basic flow is parity invariant, that is, possesses a center of symmetry. The eddy viscosity is in general a fourth-order tensor, for which a compact representation is provided. Explicit expressions of the eddy-viscosity tensor are given (i) for basic flow with low Reynolds numbers, and (ii) when the basic flow is layered, i.e., depends only on one space coordinate and time. A special class of layered flow is two-dimensional, time-independent parallel periodic flow, an example of which is the Kolmogorov flow. Such parallel flow acquires a negative-viscosity instability to large-scale perturbations transverse to the basic flow when the molecular viscosity becomes less than the r.m.s. value of the stream function of the basic flow. For flows presenting less symmetry than the Kolmogorov flow, the first large-scale instability is usually found not to be transverse, thus breaking the spatial periodicity of the basic flow. Such nontransverse instabilities, observed in a lattice-gas simulation on the Connection Machine, are reported in the companion paper by Hénon and Scholl (following paper, *Phys. Rev. A* **43**, 5365 (1991)).

Dubrulle, B., U. Frisch, M. Hénon, and J.-P. Rivet. Low viscosity lattice gases, *Physica D* **47**:27–29 (1991).
New three-dimensional lattice gas models with very low (and possibly negative) viscosities are studied theoretically and tested in numerical implementations.

Dubrulle, B., U. Frisch, M. Hénon, and J.-P. Rivet. Low-viscosity lattice gases, *J. Stat. Phys.* **59**:1187–1226 (1990).
A class of lattice gas models are studied which are variants of the "FCHC model." The aim is to achieve the highest possible Reynolds coefficient (inverse nondimensionalized viscosity) for efficient simulations of the three dimensional incompressible Navier–Stokes equations. The models include an arbitrary number of rest particles and violation of semi-detailed balance. Within the framework of the Boltzmann approximation exact expressions are obtained for the Reynolds coefficients. The minimization of the viscosity is done by solving a Hitchcock-type optimization problem for the fine-tuning of the collision rules. When the number of rest particles exceeds one, there is a range of densities at which the viscosity takes negative values. Various optimal models with up to 26 bits per node have been implemented on a CRAY-2 and their true transport coefficients have been measured with good accuracy. Fairly large discrepancies with Boltzmann values are observed when semi-detailed balance is violated; in particular, no negative viscosity is obtained. Still, the best model has a Reynolds coefficient of 13.5, twice that of the best previously implemented model and thus is about 16 times more efficient computationally. Suggestions are made for further improvements. It is proposed to use models with very high Reynolds coefficients for sub-grid-scale modeling of turbulent flows.

Dufty, James. Time correlation functions and hydrodynamic modes for lattice gas cellular automata, in *Microscopic Simulations of Complex Flow*, M. Mareschal, ed. (Plenum Press, New York, 1990), pp. 257–266.
(No abstract)

Eggert, Kenneth, Shiyi Chen, Bryan Travis, Daryl Grunau, Eugene Loh, and Frank Kovarik. Simulation of pore scale porous media flow using lattice gas methods, in *Proceedings of SPE/UH Emerging Technologies Conference, July 5–7, 1990*, (1990), pp. 269–279.
(No abstract)

Elton, B. H., C. D. Levermore, and G. H. Rodrigue. Stability of lattice Boltzmann methods, in International Symposium on Computational Fluid Dynamics, Davis, California, preprint (1991).

Elton, B. H., C. D. Levermore, and G. H. Rodrigue. Lattice Boltzmann methods for some 2-D nonlinear diffusion equations: Convergence theory, preprint (1991).

Elton, Bracy H. A numerical analysis of lattice gas and lattice Boltzmann methods in the computation of solutions to nonlinear advective-diffusive systems, Ph.D. Thesis, University of California, Davis, California (1990).
This dissertation introduces a numerical theory for the massively parallel lattice gas and lattice Boltzmann methods for computing solutions of nonlinear advective-diffusive systems. The analysis covers convergence of the methods for periodic domains in two spatial dimensions. The convergence theory includes the discrete Chapman–Enskog expansion in obtaining consistency, and conditions of monotonicity in establishing stability. Convergence of some lattice methods is studied, including two for some two-dimensional nonlinear diffusion equations, one for the one-dimensional lattice method of [B. Boghosian and C. D. Levermore, *Complex Systems*/**1**(1), 1987] for the one-dimensional Burgers equation, and one for a nonlinear two-dimensional advection-diffusion equation. Convergence is formally proven for the first three methods, revealing that they are second order accurate, conservative, conditionally monotone finite difference methods. Computational results for all the lattice methods is presented that supports the theoretical results. In addition, a domain decomposition method using mesh refinement is presented for lattice gas and lattice Boltzmann methods. Computational evidence for lattice gas methods is reported, as the domain decomposition strategy is applied to a lattice gas for the one-dimensional viscous Burgers equation.

Elton, Bracy H., C. David Levermore, and Garry H. Rodrigue. Lattice Boltzmann methods for some 2-D nonlinear diffusion equations: Computational results, in *Proceedings of the Workshop on Asymptotic Analysis and Numerical Solution of PDEs* (Argonne National Laboratory), H. Kaper, ed. (Marcel Dekker, New York, 1990), p. 197.
In this paper the authors examine two lattice Boltzmann methods (that are a derivative of lattice gas methods) for computing solutions to two two-dimensional nonlinear diffusion equations of the form

$$\frac{\partial u}{\partial t} = \nu \left(\frac{\partial D(u)}{\partial x} \frac{\partial u}{\partial x} + \frac{\partial D(u)}{\partial y} \frac{\partial u}{\partial y} \right)$$

where $u = u(\mathbf{x}, t)$, $\mathbf{x} \in R^2$, ν is a constant, and $D(u)$ is a nonlinear term that arises from a Chapman–Enskog asymptotic expansion. In particular, the authors provide computational evidence supporting recent results [B. Elton, "A Numerical Analysis of Lattice Gas and Lattice and Lattice

Boltzmann Methods in the Computation of Solutions to Nonlinear Advective-Diffusive Systems," Ph.D. dissertation, University of California, Davis, September 1990.] showing that the methods are second order convergent (in the L_1-norm), conservative, conditionally monotone finite difference methods. Solutions computed via the lattice Boltzmann methods are compared with those computed by other explicit, second order, conservative, monotone finite difference methods. Results are reported for both the L_1- and L_∞-norms.

Elton, Bracy H., and Garry H. Rodrigue. Sub-structuring for lattice gases, in *Third International Symposium on Domain Decomposition Methods for Partial Differential Equations* (SIAM, 1990), pp. 451–461.
In this paper the authors apply domain decomposition techniques to lattice gases. The authors demonstrate how a lattice gas can be modeled by a nonlinear partial differential equation using the same classical techniques as were used by Chapman and Enskog in approximating the kinetics of a real gas. As an example, the authors show how a 1-dimensional viscous Burgers' equation models a specific lattice gas. The authors then use the domain decomposition ideas for solving this differential equation to develop a substructuring technique for this exemplary lattice gas.

Ernst, M. H., and Das, S. P. Thermal cellular automata fluids, *J. Stat. Phys.* **66**:465 (1992).
The concepts of local temperature and local thermodynamic equilibrium are introduced in the context of lattice gas cellular automata (LGCAs) whose dynamics conserve energy. Green–Kubo expressions for thermal transport coefficients, in particular for the heat conductivity, are derived in a form equivalent to those for continuous fluids. All thermal transport coefficients are evaluated in Boltzmann approximation as thermal averages of matrix elements of the inverse Boltzmann collision operator, fully analogous to the results for continuous fluids, and fully model-independent. The collision operator is expressed in terms of transition probabilities between in- and out-states. Staggered diffusivities arising from spuriously conserved quantities in LGCAs are also calculated. Examples of models with either cubic or hexagonal symmetries are discussed, where particles may or may not have internal energies.

Ernst, M. H. Nonequilibrium statistical mechanics of cellular automata fluids, in *Liquids, Freezing and the Glass Transition, Les Houches 1989*, D. Levesque, J. P. Hansen, and J. Zinn-Justin, eds. (Elsevier, Amsterdam, 1991), pp. 43–143.
(No abstract)

Ernst, M. H. Temperature and heat conductivity in cellular automata fluids, in *Proceedings Euromech Colloquium 267. Series on Advanced Mathematics for Applied Sciences*, A. S. Alves, ed. (World Scientific, Singapore, 1991), pp. 186–197.
After introduction of the concept, *temperature*, consistent with thermodynamics and irreversible thermodynamics, Green–Kubo formulas are derived for the heat conductivity and the viscosities and evaluated in the Boltzmann approximation. The bulk viscosity vanishes identically. The conservation laws determine which gradients of thermodynamic variables should be considered as driving forces, and guarantee transport coefficients consistent with irreversible thermodynamics.

Ernst, M. H. Mode coupling theory and tails in CA-fluids, *Physica D* **47**:198–211 (1991).
After a summary of important effects of mode coupling theory in continuous fluids, the theory is extended to CA-fluids and the long time tails calculated for the velocity correlation function (see accompanying paper by M. van der Hoef for computer simulations) and for the stress–stress correlation function, including the spurious contributions from the staggered momentum densities. At finite densities, the Fermi statistics strongly suppresses the long time singularities arising from two fluid modes, but not those from tagged particle diffusion.

Ernst, M. H. Lattice gas cellular automata beyond the Boltzmann equation, in *Ordering Phenomena in Condensed Matter Physics* (26th Karpacz Winter School of Theoretical Physics), Z. M. Galasiewicz and A. Pekalski, eds. (World Scientific, Singapore, 1991), p. 291.

Ernst, M. H., and T. Naitoh. Self-diffusion in CA fluids, *J. Phys. A* **24**:2555–2564 (1991).
Tagged particle properties, such as the diffusion coefficients and velocity autocorrelation function are calculated in the mean-field approximation for all standard lattice gas cellular automata defined on (hyper) cubic, square and triangular lattices and on a line. Tagged particle dynamics is introduced through maximally random or minimally random collision rules. For a completely filled lattice the former reduces to a random walk, the latter to ballistic motion.

Ernst, M. H. Cellular automata in fluid dynamics, in *Fundamental Problems in Statistical Mechanics VII* (Proceedings Altenberg Summer School-1989), H. van Beijeren, ed. (North-Holland, Amsterdam, 1990), p. 321.

Ernst, M. H., and J. W. Dufty. Hydrodynamics and time correlation functions for cellular automata, *J. Stat. Phys.* **58**(1/2):57–86 (1990); erratum **61**:505 (1990).
Hydrodynamic excitations in lattice gas cellular automata are described in terms of equilibrium time correlation functions for the local conserved variables. For large space and time scales the linearized hydrodynamic equations are obtained to Navier–Stokes order. Exact expressions for the associated susceptibilities and transport coefficients are identified in terms of correlation functions. The general form of the time correlation functions for conserved densities in the hydrodynamic limit is given and illustrated by some examples suitable for comparison with computer simulation. The transport coefficients are related to time correlation functions for the conserved fluxes in a way analogous to the Green–Kubo formulas for continuous fluids. The general results are applied to a one-component fluid and several types of binary diffusion. Also discussed are the effects of unphysical slow modes, such as staggered particle and momentum densities.

Eyink, G., J. L. Lebowitz, and H. Spohn. Lattice gas models in contact with stochastic reservoirs: Local equilibrium and relaxation to the steady state, *Comm. Math. Phys.* **140**:119–131 (1991).
Extending the results of a previous work, the authors consider a class of discrete lattice gas models in a finite interval whose bulk dynamics consists of stochastic exchanges which conserve the particle number, and with stochastic dynamics at the boundaries chosen to model infinite particle reservoirs at fixed chemical potentials. The authors establish here the local equilibrium structure of the stationary measure for these model. Further, the authors prove as a law of large numbers that the time-dependent empirical density field converges to a deterministic limit process which is the solution of the initial-boundary value problem for a nonlinear diffusion equation.

Eyink, G., J. L. Lebowitz, and H. Spohn. Hydrodynamics of stationary non-equilibrium states for some stochastic lattice gas models, *Comm. Math. Phys.* **132**:253–283 (1990).
We consider discrete lattice gas models in a finite interval with stochastic jump dynamics in the interior, which conserve the particle number, and with stochastic dynamics at the boundaries chosen to model infinite particle reservoirs at fixed chemical potentials. The unique stationary measures of these processes support a steady particle current from the reservoir of higher chemical potential into the lower and are non-reversible. We study the structure of the stationary measure in the hydrodynamic limit, as the microscopic lattice size goes to infinity. In particular, we prove as a law of

large numbers that the empirical density field converges to a deterministic limit which is the solution of the stationary transport equation and the empirical current converges to the deterministic limit given by Fick's law.

Fahner, Gerald. A multispeed model for lattice-gas hydrodynamics, *Complex Systems* **5**:1–14 (1991).
A discrete model for two-dimensional hydrodynamics is presented. Compared to previous cellular-automata constructions, it has a richer spectrum of states and is thus closer to molecular dynamics. First, the model is tested regarding equilibrium isotropy. Next, thermal effects in equilibrium are discussed. Then the lattice gas is used to model the two-dimensional incompressible Navier–Stokes equation by performing a Poiseuille flow experiment. The expected effect of the system size on viscosity is found. For the shear flow the authors observe a breakdown of isotropy—much stronger than that of the equilibrium distribution—appearing as a direction-dependent viscosity. The viscosity is computed from the nonequilibrium distributions, and agreement with the simulation results is found.

Flekkøy, E. G., J. Feder, and T. Jøssang. A lattice gas simulations of osmosis, *J. Stat. Phys.* **68**:515–532 (1992).
An analysis of the phenomenon of osmosis within the lattice gas model is presented. The model considered is a two-species version of the Frisch, Hasslacher, and Pomeau model with rest particles and a semipermeable membrane which is implemented as a boundary that blocks one species, but lets the other pass freely. In this way, the equilibrium between a pure and a mixed subsystem can be studied. Analytic expressions for both the pressure difference and the fluctuations of this quantity are obtained from the entropy function for the lattice gas, and we find that these results agree well with those obtained from simulation. The osmotic flow across the membrane is studied. We characterize the concentration boundary layer, and an analytic expression for the permeability as a function of porosity is compared with results from simulations.

Frenkel, D. Fast algorithms for slow processes in lattice-gas cellular automata, *Int. J. Mod. Phys. C* **2**:66–74 (1990).
The accurate numerical study of long-time tails in time-correlation functions requires large amounts of computer time. In some cases, the necessary calculations are too time-consuming to be carried out even on present-day (super)computers. However, if one considers "lattice-gas" versions of the same problems, then it turns out that for certain problems, a speed-up of 6–10 orders of magnitude can be achieved using a very simple algorithm. As a result, one can now test theoretical (mode-coupling) predictions for long-time tails with unprecedented accuracy.

Frenkel, Daan, and M. van der Hoef. A test of mode-coupling theory, in *Microscopic Simulations of Complex Flow*, M. Mareschal, ed. (Plenum Press, New York, 1990), pp. 279–290.
(No abstract)

Frisch, U. Relation between the lattice Boltzmann equation and the Navier–Stokes equations, *Physica D* **47**:231–232 (1991).
It is shown that the lattice gas Boltzmann equation may be rewritten in a form which brings out its close relation with the Navier–Stokes equations. Various consequences are pointed out.

Gabetta, E. On a Broadwell-like lattice in a box, in *Proceedings Euromech Colloquium 267. Series on Advanced Mathematics for Applied Sciences*, A. S. Alves, ed. (World Scientific, Singapore, 1991), pp. 218–229.
The authors find conditions under which a discrete lattice introduced converges for a finite time to the plane Broadwell model in a square box.

Gabetta, E., and R. Monaco. The discrete Boltzmann equation for gases with bi-molecular chemical reactions, in *Proceedings Euromech Colloquium 267. Series on Advanced Mathematics for Applied Sciences*, A. S. Alves, ed. (World Scientific, Singapore, 1991), pp. 22–34.
The discrete Boltzmann equation for a mixture of four gases undergoing chemical reactions of bi-molecular type is derived. Thermodynamical equilibrium for such gases is investigated, deriving from the kinetic equations the mass-action law.

Gatignol, R. Constitutive laws for discrete velocity gases, in *Proceedings of the 17th International Symposium on Rarefied Gas Dynamics*, Beylich, ed. (VCH, 1991), pp. 819–829,
We generalize the discrete kinetic theory by introducing the multiple collisions: the purpose is to reduce the number of summational invariants and, if possible, to obtain the physical invariants, mass, momentum and energy, as the only ones. For a class of models, with properties of isotropy and for which the summational invariants reduce to the physical ones, we have a good agreement between the Navier–Stokes equations associated with the model and the classical equations for Newtonian fluids. In particular cases, the viscosity and the thermal conductivity coefficients are given explicitly.

Gonzales-Miranda, J. M., and J. Marro. Monte Carlo study of the generalized reaction-diffusion lattice-gas model system, *J. Stat. Phys.* **61**:1283 (1990).
The reaction-diffusion lattice-gas model is an interacting particle system out of equilibrium whose microscopic dynamics is a combination of Glauber (reaction) and Kawasaki (diffusion) processes; the Glauber rate

$c(s\mathbf{x})$ at site $\mathbf{x}$ when the configuration is s satisfies detailed balance at temperature, T, while the Kawasaki rate $\Gamma c(s; x, y)$ between nearest-neighbor sites $\mathbf{x}$ and $\mathbf{y}$ satisfies detailed balance at a different temperature, T'. The authors report on the phase diagram of that system as obtained from a series of Monte Carlo simulations of steady states in two-dimensional lattices with arbitrary values for T', T, and Γ. This generalizes previous analytical and numerical studies for $\Gamma \to \inf$ and/or $T' \to \inf$. When the rates are implemented by the Metropolis algorithm, the system is observed to undergo various types of first- and second-order (nonequilibrium) phase transitions, e.g., one may identify Onsager (equilibrium) as well as Landau (mean-field) types of continuous phase transitions.

Grosfils, P., J.-P. Boon, and P. Lallemand. Spontaneous fluctuation correlations in thermal lattice gas automata, *Phys. Rev. Lett.* **68**, 1077–1080 (1992).

Gunstensen, A. K., and D. H. Rothman. Microscopic modeling of immiscible fluids in three dimensions by a lattice-Boltzmann method, *Europhys. Lett.*, in press (1992).
The authors introduce a lattice-Boltzmann model for the simulation of two immiscible fluids in three dimensions. The model is an extension of ideas used in the construction of a previous two-dimensional immiscible lattice-Boltzmann model. The authors derive a theoretical value of the surface tension from consideration of the microscopic collision rules and verify this value with measurements from simulations.

Gunstensen, Andrew K., Daniel H. Rothman, Stephane Zaleski, and G. Zanetti. Lattice Boltzmann model of immiscible fluids, *Phys. Rev. A* **43**:4320–4327 (1991).
The authors introduce a lattice Boltzmann model for simulating immiscible binary fluids in two dimensions. The model, based on the Boltzmann equation of lattice-gas hydrodynamics, incorporates features of a previously introduced discrete immiscible lattice-gas model. A theoretical value of the surface-tension coefficient is derived and found to be in excellent agreement with values obtained from simulations. The model serves as a numerical method for the simulation of immiscible two-phase flow; a preliminary application illustrates a simulation of flow in a two-dimensional microscopic model of a porous medium. Extension of the model to three dimensions appears straightforward.

Gunstensen, A. K., and D. H. Rothman. A lattice-gas model for three immiscible fluids, *Physica D* **47**:47–52 (1991).
Lattice-gas methods have recently proven very useful for the study of immiscible mixtures of two fluids, with applications ranging from two-

phase flow in porous media to spinodal decomposition of binary fluids. Whereas the original one-phase lattice gas models the fluid as a collection of identical particles, in the immiscible two-phase lattice gas the particles are colored red or blue and the collisions between particles are chosen to achieve surface tension. The authors introduce a new lattice-gas model which extends the two-phase immiscible lattice gas to the simulation of a mixture of three immiscible fluids, i.e., red, green and blue. This extension achieves more than the obvious generalization: immiscible mixtures of three fluids yield phenomena that can be qualitatively different from analogous phenomena observed with two fluids. To demonstrate this point, the authors show simulations of phase separation of three immiscible fluids and three-phase flow in porous media.

Gunstensen, A. K., and D. H. Rothman. Galilean-invariant immiscible lattice gas, *Physica D* **47**:53–63 (1991).
Recently, lattice-gas methods have been introduced as a technique for the simulation of one- and two-phase fluid flow. These methods model the fluid as a collection of particles which propagate on a regular lattice and undergo collisions at the nodes of the lattice. In an asymptotic limit, lattice gases simulate the Navier–Stokes equations. However, these models suffer from a lack of Galilean invariance. An important physical manifestation of the lack of invariance is that the fluid vorticity advects with a velocity different from the velocity of the fluid. The authors introduce a new, Galilean-invariant, model for simulating immiscible two-phase flow. Unlike previous Galilean-invariant models, the collisions in this new model satisfy semi-detailed balance, which is achieved by the inclusion of a large number of rest particles with zero velocity. Since adding many rest particles is not computationally tractable, the presence of a large number of such particles is simulated by weighting the outcome of the collisions by a factor related to the frequency with which the collisions would have occurred if the rest particles had been explicitly included in the model. The authors demonstrate that, in the new model, the vorticity advects at the same velocity as the fluid. The authors also show that the model obeys Laplace's formula for surface tension and demonstrate an application of the new model to the Rayleigh–Taylor instability. Growth rates as a function of wavenumber computed in the early stages of the instability compare well to theoretical predictions.

Hasslacher, Brosl, and David A. Meyer. Lattice gases and exactly solvable models, *J. Stat. Phys.* **68**:575–590 (1992).
We detail the construction of a family of lattice gas automata based on a model of 't Hooft, proceeding by use of symmetry principles to define first the kinematics of the model and then the dynamics. A spurious conserved

quantity appears; we use it to effect a radical transformation of the model into one whose spacetime configurations are equivalent to the two-dimensional states of an exactly solvable statistical mechanics model, the symmetric eight-vertex model with parameters restricted to a disorder variety. We comment on the implications of this identification for the original lattice gas.

Hasslacher, B. Spontaneous curvature in a class of lattice gas field theories, *Physica D* **47**:19–26 (1991).
The authors describe a class of cellular automata having a natural lattice gas interpretation which also develop nonperturbative curvature singularities. Variations of these models could be useful in describing curvature transitions in crystals, membranes and superconducting materials.

Hayot, F. Reynolds stresses in a lattice gas, *J. Stat. Phys.*, this issue (1992).
I use a previously proposed algorithm, based on Lévy walks, to calculate and discuss longitudinal and transverse velocity correlations in turbulent channel flow. The general approach is that of lattice gas hydrodynamics.

Hayot, F. Fingering instability in a lattice gas, *Physica D* **47**:64–71 (1991).
The author describes work done over the last two years concerning a Saffman–Taylor-type instability in lattice gas hydrodynamics. The emergence of typical macroscopic laws, such as Darcy's and Laplace's, from a microscopic lattice gas is shown. The successful modeling of a fingering instability between two immiscible fluids hinges on the development of an appropriate interface algorithm.

Hayot, F. Levy walk in lattice-gas hydrodynamics, *Phys. Rev. A* **43**:806 (1991).
In order to model turbulent channel flow, and establish a closure approximation in lattice-gas hydrodynamics, the author implements a Lévy walk at the microscopic level. The algorithm is described and discussed, and results on velocity profile flattening and its shape are presented.

Hénon, M. Implementation of the FCHC lattice gas model on the Connection Machine, *J. Stat. Phys.* **68**:353–378 (1992).
The 4-dimensional FCHC lattice gas model has been implemented on a Connection Machine CM-2 with 16-K processors. Symmetries are used to reduce the collision table to a size that fits into local memory. This method avoids the degradation of the Reynolds coefficient R_*, but at the price of increased computing time. Bit shuffling between parallel lattices is introduced to reduce the discrepancy between measured viscosities and those

predicted from the Boltzmann approximation. Thereby a model with a negative shear viscosity is obtained: a fluid having a uniform initial velocity is unstable and organized nonuniform motions develop. Because of the buildup of very strong correlations between the parallel lattices, the discrepancy with the Boltzmann values decreases only very slowly with the number of parallel lattices.

Hénon, Michel, and Hans Scholl. Lattice-gas simulation of a nontransverse large-scale instability for a modified Kolmogorov flow, *Phys. Rev. A* **43**: 5365–5366 (1991).
In a companion paper, Dubrulle and Frisch [preceding paper, *Physical Review A* **43**, 5355 (1991)] develop a general formalism to determine eddy viscosities for incompressible flow. In particular, they predict a nontransverse instability for a modified Kolmogorov flow. The authors confirm quantitatively this prediction with the help of lattice-gas simulations on a Connection Machine.

Higuera, F. J., S. Succi, and R. Benzi. CFD with the lattice Boltzmann equation, in *Microscopic Simulations of Complex Flow*, M. Mareschal, ed. (Plenum Press, New York, 1990), pp. 71–84.
We review recent developments of the lattice Boltzmann Equation method (LBE) for incompressible hydrodynamics. Modifications of the discrete Boltzmann equation for a lattice gas to improve its efficiency as a numerical method are discussed. Estimations of the minimum lattice size necessary for high Reynolds number simulations are given, showing that this minimum arises from physical properties of the flows (range of scales to resolve) and not from any intrinsic limitation of the lattice gas method. Applications of the LBE to several problems are presented.

Holme, Richard, and Daniel H. Rothman. Lattice-gas and lattice-Boltzmann models of miscible fluids, *J. Stat. Phys.* **68**: 409–430 (1992).
We introduce new lattice-gas and lattice-Boltzmann models for simulating miscible fluids in two dimensions. The inclusion of a nonlocal interaction produces a lattice gas with lower diffusivity than achieved before. To overcome some observed unphysical properties of this lattice gas, we introduce a lattice-Boltzmann analogue of the model. We first formulate a miscible two-component lattice-Boltzmann model with local interactions only, and show that its diffusivity is determined by an eigenvalue of the linearized collision operator. Diffusivity is then reduced by including nonlocal interactions. The utility of the model is demonstrated by a simulation of two-dimensional viscous fingering.

Illner, R. Solutions of the steady Boltzmann equation in a slab: Applied problems, pure results, in *Proceedings Euromech Colloquium 267. Series on Advanced Mathematics for Applied Sciences*, A. S. Alves, ed. (World Scientific, Singapore, 1991), pp. 104–112.
The objective of this article is to present recent progress on a paradigmatic boundary value problem for the steady Boltzmann equation. A comparison with older results for discrete velocity models is also done, and some open problems are suggested.

Jensen, Henrik Jeldtoft. Lattice gas as a model of $1/f$ noise, *Phys. Rev. Lett.* **6**:3103–3106 (1990).
Direct numerical measurement of the power spectrum of the number of particles on the lattice demonstrates in an example of probably broad physical relevance that $1/f$ behavior can arise due to self-organized criticality. Different versions of the model are studied in order to look for universality.

Kapral, Raymond, Anna Lawniczak, and Paul Masiar. Reactive dynamics in a multi-species lattice-gas automaton, *J. Chem. Phys.* **96**:2762–2776 (1992).
A multi-species reactive lattice-gas automaton model is constructed and used to study chemical oscillations and pattern formation processes in a spatially-distributed two-dimensional medium. Both steady state and oscillatory dynamics are explored. Nonequilibrium spatial structures are also investigated. The automaton simulations show the formation of rings of chemical excitation, spiral waves and Turing patterns. Since the automaton model treats the dynamics at a mesoscopic level, fluctuations are included and nonequilibrium spatial structures can be investigated at a deeper level than reaction-diffusion equation descriptions.

Kapral, Raymond, Anna Lawniczak, and Paul Masiar. Oscillations and waves in a reactive lattice-gas automaton, *Phys. Rev. Lett.* **66**:2539–2542 (1991).
A lattice-gas automaton model is constructed for multispecies, chemically reacting, spatially distributed systems and applied to a two-species reaction. The automaton simulations show monotone and oscillatory decay to the steady state as well as excitability and limit cycles. Chemical waves, such as rings and spiral waves, and Turing patterns that arise from the bifurcation of the homogeneous state are found. The model allows the exploration of nonequilibrium spatial structures at the mesoscopic level and goes beyond the usual reaction-diffusion equation descriptions.

Kawashima, S. Asymptotic behavior of solutions to the discrete Boltzmann equation, in *Proceedings Euromech Colloquium 267. Series on Advanced*

Mathematics for Applied Sciences, A. S. Alves, ed. (World Scientific, Singapore, 1991), pp. 35–44.
(No abstract)

Kirkpatrick, T. R., and Ernst, M. H. Kinetic theory for lattice gas cellular automata, *Phys. Rev. A* **44**:8051 (1991).
The kinetic theory for lattice gas cellular automata is extended beyond Boltzmann's mean field approximation by including correlated ring-type collisions. This theory provides explicit expressions for time-correlation functions for all times in terms of a ring collision integral. We also obtain some exact results for time correlation functions at short times. In particular, deviations from the Boltzmann equation result observed in computer simulations of the velocity-autocorrelation function of three-dimensional systems after two time steps are explained. For long times the results obtained reduce to those found from the phenomenological mode-coupling theory.

Koelman, J. M. V. A. A simple lattice Boltzmann scheme for Navier–Stokes fluid flow, *Europhys. Lett.* **15**:603–607 (1991).
A lattice Boltzmann algorithm for the computation of incompressible Navier–Stokes flow is presented. This algorithm can be written down in a simple, explicit form for a general class of lattices. By working consistently within a Boltzmann description, the model is free from ambiguities and inconsistencies. It automatically gives rise to isotropic, Galilean-invariant flow behavior for any regular 2D or 3D lattice of sites.

Kohring, G. A. An efficient HDCA for simulating fluids with large viscosities, *J. Stat. Phys.* **66**:1177–1184 (1992).
A hydrodynamical cellular automata (HDCA) for simulating two-dimensional fluids with large viscosities is proposed. The model is characterized by a mean-free path which is of the same size as in the FHP-III model, but with a viscosity more than ten times larger. This new model should make simulations of flows at low Reynolds number more efficient.

Kohring, G. A. Calculations of drag coefficients via hydrodynamic cellular automata, *J. Phys. II* **2** (1992).
The drag coefficient, C_D, of an arbitrary shaped object can be calculated by two-dimensional hydrodynamic cellular automata. Results spanning nearly four orders of magnitude in the Reynolds number ($0.1 < Re < 10^3$) are presented for a simple, hexagonal object, and good quantitative agreement with previous experiments on cylinders is obtained.

Kohring, G. A. Effect of finite grain size on the simulation of fluid flow in porous media, *J. Phys. II* **1**:87–90 (1991).
Effects caused by the necessarily finite grain size used in simulations of flow

in porous media are systematically studied in two dimensional hydrodynamic cellular automata with systems of up to 88 million sites. The permeability of the media, K, is found to be a function of the grain size, R, and an extrapolation to physically realistic grain sizes is given.

Kohring, G. A. Limitations of a finite mean free path for simulating flows in porous media, *J. Phys. II* **1**:593–597 (1991).
When the mean free path, λ, of fluid particles for Hydrodynamic Cellular Automata is not much smaller than the characteristic length of the system, then hydrodynamic correlations do not have a chance to develop and true hydrodynamic flow will not be obtained. By studying a simple two dimensional system, it is concluded that the finite size corrections to the permeability, κ, for pore size, R, are of the form: $1 + 7 \cdot (\lambda/R)$. The limitations this result places on the use of such methods for studying flows in porous media are discussed.

Kohring, G. A. Parallelization of short- and long-range cellular automata on scalar, vector, SIMD and MIMD machines, *Int. J. Mod. Phys. C* **2**:755–772 (1991).
Algorithms exhibiting parallelization on many different levels are discussed for short and long range cellular automata implemented on scalar, vector, SIMD and MIMD machines. Short range cellular automata are commonly used for simulating hydrodynamic fluid flows, while long range cellular automata are applicable to neural networks at zero temperature. A common programming approach based upon multi-spin coding and including higher levels of parallelization when possible, has been used to implement these models on the SUN SPARC-1, the IBM-3090, the Alliant FX/2800, the NEC-SX3/11, the Cray-YMP/832 and the Connection Machine, CM-2. Section four of the paper compares the performance of these computers for the algorithms discussed in the text. Additionally, the major subroutines for each computer type are given in the appendix.

Kohring, G. A. Using cellular automata for modeling fluid flows in porous media, Invited talk presented at the Seminar I Petroleumsfysikk, Stavanger, Norway (15–16 August, 1991).
The fundamental aspects of modeling fluid flows in porous media using cellular automata are discussed. Efficients methods for simulating these models on vector, SIMD and MIMD machines are presented. Results for systems with up to 200 million particles show unique finite size effects which can be interpreted as arising from the quite large mean free path, λ, of the fluid particles. Empirically, we find these finite size effects to be proportional to: $1 + 7 \cdot \lambda/R$, where R is the characteristic size of the system. Using this information, we estimate the dependence of the permeability, κ,

on the porosity, ϕ, of a 2-D porous medium as: $\kappa \propto e^{6.5 \cdot \phi}/(1-\phi)$. Finally, in order to improve the efficiency of low Reynolds number simulations, a new model is presented which has a much larger viscosity than previous models.

Kohring, G. A. Calculation of the permeability of porous media using hydrodynamic cellular automata, *J. Stat. Phys.* **63**:411–418 (1991).
The permeability of two-dimensional porous media is calculated numerically as a function of porosity using the hydrodynamic cellular automata (lattice gas) approach. Results are presented for systems with up to 22 million sites (8192*2688). For randomly distributed solid obstacles whose macroscopic dimensions are much longer than the mean free path of particles in the fluid, the permeability, κ, varies with porosity, ε, as $\kappa \propto (\varepsilon - 0.6)/(1-\varepsilon)$ for $\varepsilon > 0.7$. When the solid obstacles are much smaller than the mean free path of particles in the fluid, i.e., when they form a dust of point objects, then such a relationship no longer holds and the permeability is more than an order of magnitude smaller than for the former case. The program used for the simulations is discussed and a listing is presented.

Kong, X. P., and E. G. D. Cohen. A kinetic theorist's look at lattice gas cellular automata, *Physica D* **47**:9–18 (1991).
The diffusion behavior of a number of Lorentz lattice gases is studied in its dependence on collision rules and its similarity to corresponding Lorentz gases that are continuous in space, but have the same discrete velocity space. The difference in behavior resulting from probabilistic or deterministic collision rules is discussed.

Kong, X. P., and E. G. D. Cohen. Diffusion and propagation in triangular Lorentz lattice gas cellular automata, *J. Stat. Phys.* **62**:737–757 (1991).
The diffusion process of point particles moving on regular triangular and random lattices, randomly occupied with stationary scatterers (a Lorentz lattice gas cellular automaton), is studied, for strictly deterministic scattering rules, as a function of the concentration of the scatterers. In addition to the normal and various kinds of retarded diffusion found before on the regular square lattice, straight-line propagation through the scatterers is observed.

Kong, X. P., and E. G. D. Cohen. Lorentz lattice gases, abnormal diffusion and polymer statistics, *J. Stat. Phys.* **62**:1153 (1991).
Diffusive behavior in various Lorentz lattice gases, especially wind-tree-like models, is discussed. Comparisons between lattice and continuum models as well as deterministic and probabilistic models are made. In one deterministic model, where the scatterers behave like double-sided mirrors, a

new kind of abnormal diffusion is found, viz., the mean square displacement is proportional to the time, but the probability density distribution function is non-Gaussian. The connections of this mirror model with the percolation problem and the statistics of polymer chains on a lattice are also discussed.

Kougias, Ch. F., G. Krause, and A. Rauh. Simulation of river-discharge fronts with lattice gas automata, in *Proceedings Euromech Colloquium 267. Series on Advanced Mathematics for Applied Sciences*, A. S. Alves, ed. (World Scientific, Singapore, 1991), pp. 156–165.
An extended FHP lattice gas model with two kinds of particles is introduced in order to simulate the dynamics of a frontal interface between a salt and fresh water body. First, the hydrodynamical similarity has been checked for the given lattice gas flow whereby the overall Richardson number, *Ri*, is verified to be the governing dimensionless parameter. From the time development of the flow pattern, it is examined how the convergence of the flow is built up and how the stability of the front and its velocity depend on *Ri*.

Ladd, A. J. C. Hydrodynamic interactions and transport coefficients in a suspension of spherical particles, in *Microscopic Simulations of Complex Flow*, M. Mareschal, ed. (Plenum Press, New York, 1990), pp. 129–140.
Particulate suspensions of solids in liquids can be understood in terms of the microstructure of the solid phase by using the well-known techniques of numerical statistical mechanics. The major problem with such an approach has been the incorporation of the long-range, many-body hydrodynamic forces between the suspended particles. In this paper, I describe a general computational method for calculating the forces and torques exerted by slowly moving spheres suspended in an incompressible fluid. The method can be used to determine bulk constitutive properties of solid–fluid suspensions or particulate porous media. Numerical results for the sedimentation velocity and high frequency viscosity of monodisperse suspensions have been obtained, and the results are shown to compare very well with experimental measurement.

Ladd, Anthony J. C., and Daan Frenkel. Dissipative hydrodynamic interactions via lattice-gas cellular automata, *Phys. Fluids A* **2**:1921–1924 (1990).
A three-dimensional lattice-gas model has been used to determine the dissipative hydrodynamic interactions between spherical particles. When the particles are close together, the accuracy of the lattice-gas simulations is superior to typical integral-equation solutions of the creeping-flow equations. Moreover, the computational requirements scale linearly with system

size, instead of quadratically or cubically. A new set of microrules has been implemented, which simulates a constant-velocity, no-slip boundary condition at the solid–fluid surfaces. Numerical results for various drag coefficients are reported.

Lavallèe, P., J. P. Boon, and A. Noullez. Boundaries in lattice gas flows, *Physica D* **47**:233–240 (1991).
A one-dimensional lattice gas model is used to study the interaction of fluid flows with solid boundaries. Various interaction mechanisms are examined. Lattice Boltzmann simulations show that bounce-back reflection is not the only interaction that yields "no-slip" boundary conditions (zero velocity at a fixed wall) and that Knudsen-type interaction is also appropriate.

Lawniczak, A., D. Dab, R. Kapral, and J. P. Boon. Reactive lattice gas automata, *Physica D* **47**:132–158 (1991).
A probabilistic lattice gas cellular automaton model of a chemically reacting system is constructed. Microdynamical equations for the evolution of the system are given; the continuous and discrete Boltzmann equations are developed and their reduction to a generalized reaction-diffusion equation is discussed. The microscopic reactive dynamics is consistent with any polynomial rate low up to the fourth order in the average particle density. It is shown how several microscopic CA rules are consistent with a given rate law. Like most CA systems, the present one has spurious properties whose effects are shown to be unimportant under appropriate conditions. As an explicit example of the general formalism a CA dynamics is constructed for an autocatalytic reactive scheme known as the Schlögl model. Simulations show that in spite of the simplicity of the underlying discrete dynamics the model exhibits the phase separation and wave propagation phenomena expected for this system. Because of the microscopic nature of the dynamics the role of internal fluctuations on the evolution process can be investigated.

Lebowitz, J. L., E. Orlandi, and E. Presutti. A particle model for spinodal decomposition, *J. Stat. Phys.* **63**:933–974 (1991).
The authors study a one-dimensional lattice gas where particles jump stochastically obeying an exclusion rule and having a "small" drift toward regions of higher concentration. They prove convergence in the continuum limit to a nonlinear parabolic equation whenever the initial density profile satisfies suitable conditions which depend on the strength, a, of the drift. There is a critical value, a_c, of a. For $a < a_c$, the density values are unrestricted, while for $a \geqslant a_c$, they should all be to the right or to the left of a given interval $I(a)$. The diffusion coefficient of the limiting equation can be continued analytically to $I(a)$, and, in the interior of $I(a)$, it has

negative values which should correspond to particle aggregation phenomena. They also show that the dynamics can be obtained as a limit of a Kawasaki evolution associated to a Kac potential. The coefficient, a, plays the role of the inverse temperature, β. The critical value of a coincides with the critical inverse temperature in the van der Waals limit and $I(a)$ with the spinodal region. It is finally seen that in a scaling, intermediate between the microscopic and the hydrodynamic, the system evolves according to an integro-differential equation. The instanton solutions of this equation, as studied by Dal Passo and De Mottoni, are then related to the phase transition region in the thermodynamic phase diagram; analogies with the Cahn–Hilliard equations are also discussed.

Lee, S. H., and E. Y. Chung. A cellular automaton model for flow in a heterogeneous reservoir, SPE paper number 21229, presented February 17, 1991.

Levermore, D. Fluid dynamical limits of discrete kinetic theories, in *Microscopic Simulations of Complex Hydrodynamic Phenomena*, M. Mareschal and B. L. Holian, eds. (Plenum Press, New York, 1992).
The determination of fluid dynamical limits is presented for a large class of discrete kinetic theories. The formalism includes models with multi-speeds, multi-species, internal energies and many other options. The interrelationship between the concepts of equilibria, conservation, and dissipation through that of entropy is shown to be critical. This relationship is provided by an abstraction of the classical physical entropy as it is manifest in Boltzmann's classical H-theorem. In particular, it applies to a class of BGK models that is well suited for fluid dynamical simulations. Formal derivations of generalized compressible Euler and generalized incompressible Navier–Stokes systems are given. The implications of this analysis for the implementation of fluid dynamical simulations is discussed.

Liu, Fong, and Nigel Goldenfeld. Deterministic lattice model for diffusion-controlled crystal growth, *Physica D* **47**:124–131 (1991).
An efficient lattice model is developed to study the late stages of diffusion-controlled crystal growth. The authors establish the existence of a Dense Branching Morphology and its relation to the diffusion-limited aggregation. The authors find a clear morphological transition from the kinetic-effect-dominated growth to the surface-tension-dominated growth, marked by a difference in the way growth velocity scales with undercooling. The authors also study the evolution of interfacial instability and find a scaling behavior for the interface power spectra, indicating the nonlinear selection of a unique length scale.

Luo, Li-Shi, Hudong Chen, Shiyi Chen, G. D. Doolen, and Y. C. Lee. Generalized hydrodynamic transport in lattice-gas automata, *Phys. Rev. A* **43**:7097–7100 (1991).
The generalized hydrodynamics of two-dimensional lattice-gas automata is solved analytically in the linearized Boltzmann approximation. The dependence of the transport coefficients (kinematic viscosity, bulk viscosity, and sound speed) upon wave number, k, is obtained analytically. Anisotropy of these coefficients due to the lattice symmetry is studied for the entire range of wave number, k. Boundary effects due to a finite mean free path (Knudsen layer) are analyzed, and accurate comparisons are made with lattice-gas simulations.

McNamara, G. R. Diffusion in a lattice gas automaton, *Europhys. Lett.* **12**:329–334 (1990).
A two-dimensional lattice gas automaton with two species (colors) of particles is studied to determine the behavior of its diffusion coefficient. The diffusion coefficient is measured by establishing a color-density gradient across the width of a rectangular channel and observing the resulting flux of particles of the two species. Accurate estimates of the diffusion coefficient as a function of system size are obtained and are found to exhibit the logarithmic divergence expected for transport coefficients in two dimensions.

Mora, Peter. The lattice Boltzmann phononic lattice solid, *J. Stat. Phys.* **68**:591–610 (1992).
I present a Boltzmann lattice gas-like approach for modeling compressional waves in an inhomogeneous medium as a first step toward developing a method to simulate seismic waves in complex solids. The method is based on modeling particles in a discrete lattice with wavelike characteristics of partial reflection and transmission when passing between links with different properties as well as phononlike interactions (i.e., collisions), with particle speed dependent on link properties. In the macroscopic limit, this approach theoretically yields compressional waves in an inhomogeneous acoustic medium. Numerical experiments verify the method and demonstrate its convergence properties. The lattice Boltzmann phononic lattice solid could be used to study how seismic wave anisotropy and attenuation are related to microfractures, the complex geometry of rock matrices, and their couplings to pore fluids. However, additional particles related to the two transverse phonons must be incorporated to correctly simulate wave phenomena in solids.

Mora, Peter, and Bertrand Maillot. Numerical studies of the phononic lattice solid macroscopic limit, to appear (1992).
The lattice Boltzmann phononic lattice solid is a lattice gas based approach

to simulate macroscopic wave phenomena in complex solids. It models number densities of wavelike particles propagating and interacting on a discrete lattice. The particles are partially reflected and transmitted at boundaries between lattice links with different properties such as particle speed. In the macroscopic limit, the one-particle phononic lattice solid simulates compressional acoustic waves in an inhomogeneous medium. The approach could potentially be used to investigate the causes of seismic anisotropy and attenuation which are thought to be controlled by the microscopic geometry of rock matrices, microfractures, and their couplings to pore fields. Finite-lattice effects which introduce additional anisotropy into the wave speed and viscosity could bias such studies. Numerical experiments in homogeneous media are used to investigate the lattice solid macroscopic limit and when finite-lattice effects become significant. Wave speed and viscosity measurements of long-wavelength standing waves verify the theoretical predictions made in the macroscopic limit. Spectra of wavespeed and viscosity are computed by analyzing time series from simulations of standing waves at all discrete wavenumbers of a lattice. The spectra are isotropic near the origin, $k = 0$, as expected. The wavenumber at which the spectra become anisotropic suggests a limit beyond which the finite-lattice effects dominate. This limit depends strongly on particle density as well as particle speed.

Naitoh, T., and M. H. Ernst. Full time-dependence of the VACF in CA-fluids: Theory and simulations, in *Proceedings Euromech Colloquium 267. Series on Advanced Mathematics for Applied Sciences*, A. S. Alves, ed. (World Scientific, Singapore, 1991), pp. 166–175.
The velocity autocorrelation function (VACF) in a 1-D 5-bits model, the 2-D FHP-III model and the quasi 3-D FCHC model are investigated using mode coupling theory accounting for finite size corrections and for all possible pairs of hydrodynamic modes. This extended mode coupling theory describes the molecular dynamics data of Frenkel quantitatively from about three mean free times on. For times up to two mean free times, the MD data agree with the predictions from the Boltzmann approximation. However, in the quasi 3-D model, the MD results exhibit unexplained deviations in the early stages from the Boltzmann values and in the intermediate stage from those obtained with the extended mode coupling theory.

Naitoh, T., M. H. Ernst, M. A. van der Hoef, and D. Frenkel. Extended mode coupling and simulations in cellular-automata fluids, *Phys. Rev. A* **44**:2484–2494 (1991).
The velocity autocorrelation function (VACF) of lattice-gas cellular-automata fluids has been calculated by mode-coupling (MC) theory for

finite systems, including sound modes, and compared with computer simulations on small ($N \approx 10^3$) and large ($N \approx 10^6$) two- and three-dimensional (3D) systems for reduced densities, f, ranging from 0.05 to 0.8. For times, t, up to $6t_0$ (mean free times), the simulated VACF agrees with Boltzmann relaxation. In 2D the agreement with MC theory is excellent for $t \,?\, t_0$ and has been tested over intervals of several acoustic traversal times. In 3D agreement is still good, but sets in after much larger times ($150t_0$ at $f = 0.1$ and $60t_0$ at $f = 0.8$). However, there are disagreements in the smallest systems at the lowest densities, where the observed VACF at largest times is about 6% ($f = 0.1$) and 9% ($f = 0.05$) larger than the theoretical values.

Naitoh, T., M. H. Ernst, and James W. Dufty. Long-time tails in two-dimensional cellular automata fluids, *Phys. Rev. A* **42**:7187–7194 (1990).
Mode coupling theory is used to calculate the Green–Kubo time correlation functions for the 2-D FHP lattice gas cellular automaton. An intermediate algebraic decay α/t and an asymptotic decay $\alpha/[t\sqrt{\ln(t)}]$ are found. The amplitudes for these decays are calculated and it is found that the contribution from diffusive modes associated with the spurious conservation laws is significant. For the computer simulations in CA-fluids, only the algebraic tail is relevant; the asymptotic tail dominates only on time scales large compared to 10^{10} mean free times.

Nannelli, Francesca, and Sauro Succi. The lattice Boltzmann equation on irregular lattices, *J. Stat. Phys.* **68**:401–408 (1992).
A general framework to extend the lattice Boltzmann equation to arbitrary lattice geometries is presented and numerically demonstrated for the case of two-dimensional Poiseuille flow. The new scheme considerably extends the range of applicability of the Boltzmann method to problems requiring the use of nonuniform grids.

Nasilowski, R. A cellular-automaton fluid model with simple rules in arbitrarily many dimensions, *J. Stat. Phys.* **65**:97–138 (1991).
A new cellular-automaton model for fluid dynamics is introduced. Unlike the conventional FHP-type models, the model uses easily implementable, deterministic pair interaction rules which work on arbitrary-dimensional orthogonal lattices. The statistical and hydrodynamic theory of the model is developed, and the Navier–Stokes-like hydrodynamic equations that describe the macroscopic behavior of the model are derived. It turns our that the unwanted anisotropic convection behavior can be eliminated in the incompressible limit by suitable choice of the mass density. An explicit expression for the viscosity tensor is calculated from a Boltzmann-type approximation. Unfortunately, the viscosity turns out to be anisotropic,

which is a drawback as against the conventional FHP and FCHC models. Nevertheless, the new model could become interesting for fluid dynamic problems with additional variables (e.g., free surfaces), especially in two dimensions, since its simple rules could relatively easily be extended for such cases.

Noullez, Alain. Lattice gas automata: Theoretical aspects and simulations, (in French). Ph.D. dissertation, University of Brussels (1990).

Noullez, A., and J.-P. Boon. Long-time correlations in 2D lattice gas, *Physica D* **47**:212–215 (1991).
The authors present the results of CA simulations of a moderately dense lattice gas using an extended version of the FHP model for colored automata. By tracking a tagged particle, the authors construct its velocity autocorrelation function and the authors show that the corresponding power spectrum exhibits a low-frequency contribution characteristic of the long-time power law behavior ($\approx t^{-1}$, in 2D).

Olesky, C. Diffusion coefficient increases with density in a lattice-gas model, *J. Phys. A* **24**:L751–755 (1991).
The author reports computer simulations of the diffusion coefficient in a two-dimensional lattice Lorentz gas with interacting particles. The simulations show that the diffusion coefficient has a maximum as a function of the particle density in models with strongly correlated particle-scatterer collisions.

Orlandi, E., and E. Presutti. Some rigorous results on phase segregation for stochastic cellular automata, in *Proceedings Euromech Colloquium 267. Series on Advanced Mathematics for Applied Sciences*, A. S. Alves, ed. (World Scientific, Singapore, 1991), pp. 45–59.
(No abstract)

Paetzold, O. Vectorization of diffusion of lattice gas without double occupancy, *Computer Phys. Commun.* **64**:1–6 (1991).
The authors describe an algorithm for lattice-gas diffusion without double occupancy, which is completely vectorizable on computers like the CRAY. It is significantly faster than the algorithm usually used on scalar computers, which has not been vectorized until now. The use of sublattices is the clue to the vectorization of the lattice-gas diffusion model.

Piechór, K. The Couette flow by a four-velocity model of the Uehling–Uhlenbeck equation, in *Proceedings Euromech Colloquium 267. Series on Advanced Mathematics for Applied Sciences*, A. S. Alves, ed. (World Scientific, Singapore, 1991), pp. 176–185.
A plane four-velocity model of the Uehling–Uhlenbeck equation is used to study the Couette flow. Assuming the Maxwellian law of reflection of molecules from the boundaries, the authors solve the problem explicitly. Graphs representing the profiles of the mean velocity are given.

Platkowski, T. On a boundary value problem for the Carleman model of the Boltzmann equation, in *Proceedings Euromech Colloquium 267. Series on Advanced Mathematics for Applied Sciences*, A. S. Alves, ed. (World Scientific, Singapore, 1991), pp. 113–122.
Existence and uniqueness of solutions of a boundary value problem with general boundary data for the Carleman model of the Boltzmann equation are investigated. Necessary and sufficient conditions for existence of the solutions, and results of a numerical study of a trend to equilibrium of the underlining initial boundary value problem are discussed. Explicit examples of the nonunique positive solutions are given.

Preziosi, L., and E. Longo. On the decomposition of domains in non-linear discrete kinetic theory, in *Proceedings Euromech Colloquium 267. Series on Advanced Mathematics for Applied Sciences*, A. S. Alves, ed. (World Scientific, Singapore, 1991), pp. 144–155.
This paper deals with the coupling of the nonlinear heat equation with the discrete Boltzmann equation in a class of initial-boundary value problems. The starting point is the formulation of the problem, then suitable coupling equations are used in order to derive a self-consistent set of equations for the whole system.

Qian, Y. H., D. d'Humières, and P. Lallemand. Diffusion simulation with a deterministic one-dimensional lattice-gas model, *J. Stat. Phys.* **68**:653–574 (1992).
A one-dimensional lattice-gas model is proposed and used to simulate diffusion processes in one dimension. Explicit forms of transport coefficients are given as a function of density and kinetic energy within the Boltzmann approximation. Without definitions of temperature and pressure, a steady nontrivial solution is given analytically in the nonconvective case when the kinetic energy is kept constant.

Qian, Y. H., D. d'Humières, and P. Lallemand. Lattice BGK models for Navier–Stokes equation, *Europhys. Lett.* **17**(6):479–484 (1992).
We propose the lattice BGK models, as an alternative to lattice gases or the lattice Boltzmann equation, to obtain an efficient numerical scheme for the simulation of fluid dynamics. With a properly chosen equilibrium distribution, the Navier–Stokes equation is obtained from the kinetic BGK equation at the second order of approximation. Compared to lattice gases, the present model is noise-free, has Galilean invariance and a velocity independent pressure. It involves a relaxation parameter that influences the stability of the new scheme. Numerical simulations are shown to confirm the speed of sound and the shear viscosity.

Qian, Y. H., D. d'Humières, and P. Lallemand. A one-dimensional lattice Boltzmann equation with Galilean invariance, in *Advances in Kinetic Theory and Continuous Mechanics*, R. Gatignol and Soubbaramayer, eds. (Springer-Verlag, 1991), pp. 127–138.
A three-velocity one-dimensional Lattice Boltzmann Equation is presented. The stability of the equilibrium distribution is studied and the dynamical equations are given. It is shown that Galilean invariance can be recovered for the proper choice of the collision operator. This particular model is then used to compare the results of numerical simulations to the behavior of a shock tube.

Rechtman, R., and A. Salcido. Thermodynamic entropy and temperature of a nine velocities lattice gas automaton, in *Proceedings Euromech Colloquium 267. Series on Advanced Mathematics for Applied Sciences*, A. S. Alves, ed. (World Scientific, Singapore, 1991), pp. 208–217.
Using the microcanonical ensemble formalism, the authors obtain the equilibrium entropy density of a nine velocities lattice gas automaton on a square lattice. From the entropy, all the thermodynamic equilibrium properties follow but the authors focus on the temperature. Our results are exact, so that any definition of temperature used when studying the hydrodynamic behavior of the model should reduce to the thermodynamic temperature.

Riccardi, G., C. Bauer, and H. Lim. Boundary and obstacle processing in a vectorized model of lattice gas hydrodynamics, *Physica D* **47**:281–295 (1991).
The authors describe a vectorized supercomputer implementation of a cellular automaton model for lattice gas hydrodynamics. A detailed description of the algorithm is given along with a careful complexity analysis and performance evaluation of it. Particular attention is paid to boundary and obstacle processing. Two applications of the program are described: an acoustic wave model and an obstructed flow through a pipe. The results of executing these models are displayed with density maps and flow diagrams.

Rivet, J. P. Spontaneous symmetry-breaking in the 3-D wake of a long cylinder, simulated by the lattice gas method, *C. R. Acad. Sci. Paris II* **313**:151 (1991).
The author presents a direct numerical simulation by the lattice gas method of the three-dimensional non-stationary incompressible flow at a Reynolds number of 74, past a circular cylinder, with a uniform incident flow. The author describes the three-dimensional structure and the time-evolution of the wake, which leads to an oblique vortex shedding situation.

This kind of wake is not invariant under translation parallel to the cylinder axis.

Rothman, D. Complex rheology in a model of a phase-separating fluid, *Europhys. Lett.* **14**:337–342 (1991).
The time-dependent effective shear viscosity of a two-dimensional phase-separating fluid is measured by numerical simulation of a momentum-conserving lattice-gas model of an immiscible binary mixture. Simulations of phase separation in a simple shear flow reveal that the effective viscosity can be greater than 5 times the viscosity of the constituent fluids prior to mixing. The effective viscosity is strongly time-dependent, with a behavior characterized by a rapid increase (strain thickening) followed by a gradual drop-off (strain thinning) to a steady state. Explicit measurements of the time-dependent excess stress are shown to be well-correlated with analogous measurements made only from knowledge of the orientation of interfaces.

Rothman, D. Macroscopic laws for immiscible two-phase flow in porous media: Results from numerical experiments, *J. Geophys. Res.* **95**:8663–8674 (1990).
Flow through porous media may be described at either of two length scales. At the scale of a single pore, fluids flow according to the Navier–Stokes equations and the appropriate boundary conditions. At a larger, volume-averaged scale, the flow is usually thought to obey a linear Darcy law relating flow rates to pressure gradients and body forces via phenomenological permeability coefficients. Aside from the value of the permeability coefficient, the slow flow of a single fluid in a porous medium is well-understood within this framework. The situation is considerably different, however, for the simultaneous flow of two or more fluids: not only are the phenomenological coefficients poorly understood, but the form of the macroscopic laws themselves is subject to question. I describe a numerical study of immiscible two-phase flow in an idealized 2-D porous medium constructed at the pore scale. Results show that the macroscopic flow is a nonlinear function of the applied forces for sufficiently low levels of forcing, but linear thereafter. The crossover, which is not predicted by conventional models, occurs when viscous forces begin to dominate capillary forces; i.e., at a sufficiently high capillary number. In the linear regime, the flow may be described by the linear phenomenological law $u_i = \sum_j L_{ij} f_j$, where the flow rate u_i of the ith fluid is related to the force f_j applied to the jth fluid by the matrix of phenomenological coefficients, L_{ij}, which depend on the relative concentrations of the two fluids. The diagonal terms are proportional to quantities commonly referred to as "relative permeabilities." The cross terms represent viscous coupling between the two fluids; they are

conventionally assumed to be negligible, and require special experimental procedures to observe in a laboratory. In contrast, in this numerical study the cross terms are straightforward to measure and are found to be of significant size. The cross terms are additionally observed to be approximately equal, which is the behavior predicted by Onsager's reciprocity theorem. However, persistent transient effects can render the reciprocity unobservable. The numerical study is performed with a discrete numerical model of fluid mixtures called the immiscible lattice gas. The immiscible lattice gas, essentially a discrete model of the molecular dynamics of immiscible mixtures, models both the Navier–Stokes equations and surface tension. Numerical tests presented here additionally provide quantitative validation of the method's ability to simulate wetting phenomena and the effects of capillary pressure. Whereas the numerical study of the linear phenomenological laws utilizes a highly simplified porous medium with one pore and 2 throats, numerical examples of wetting and non-wetting invasion experiments in a geometrically complex 2-D porous medium are also provided.

Rothman, D. Deformation, growth, and order in sheared spinodal decomposition, *Phys. Rev. Lett.* **65**:3305–3308 (1990).
The effect of hydrodynamics on growth is studied by numerical simulation of two-dimensional phase separation in a simple shear flow. The simulations are performed with a momentum-conserving lattice-gas model of an immiscible binary fluid. The results reveal that an anisotropic anomaly that was previously observed in experimentally-obtained structure functions is due to a shear-induced, smectic-like ordering of the domains.

Scheunders, P., and J. Naudts. Long-time tail of the velocity-autocorrelation function in the Lorentz lattice gas, *Phys. Rev. A* **41**:3415–3418 (1990).
The authors present numerical results for the first and second moments of the distribution of collision times of the $d=2$ Lorentz lattice gas with density q in the range 0.2–0.8. They are used to calculate the mean-square displacement $\langle X^2(T_k)\rangle$ as a function of the number of collisions k. Using an asymptotic relation the mean-square displacement $\langle X^2(t)\rangle$ as function of time is obtained from the latter quantity. As a result the authors are able to predict, in an accurate numerical way, the long-time tail of the velocity-autocorrelation function.

Sero-Guillaume, O. E., and D. Bernardin. A lattice gases model for heat transfer and chemical reaction, *Eur. J. Mech. B Fluids* **9**(2):177–196 (1990).
A model of a multi-species, multi-speed lattice gas with energy levels is considered. Each particle can be composed of atoms, and the collisional invariants are the number of atoms of each type, the total momentum and the total energy. Using the Gibbs universal distribution, the thermo-

dynamic relations at equilibrium are studied. The evolution equations of the macroscopic quantities with invariants are derived by the Chapman–Enskog method. The ability of this kind of model to simulate thermal processes and chemical reactions at low hydrodynamic velocities is shown.

Somers, J. A., and P. C. Rem. Flow computation with lattice gases, *Appl. Sci. Res.* **48**:391–435 (1991).
Cellular automata offer a simple way to simulate flow in complex geometries. The algorithm computes flow by tracking the paths of individual particles of a simple lattice gas. An advantage of this approach is that many of the traditional problems of conventional numerical techniques in dealing with complex boundaries are avoided. In particular explicit front tracking of moving interfaces in two-phase flow is not necessary. On the other hand, some problems appear that are specific to lattice gas models propose solutions to these problems. Furthermore, the authors give an overview of the current status of lattice gas algorithms with respect to applications in fluid flow.

Somers, J. A., and P. C. Rem. Analysis of surface tension in two-phase lattice gases, *Physica D* **47**:39–46 (1991).
One of the promising fields of application for lattice gas methods is two-phase flow simulation. An important issue in the design of two-phase lattice gas models is managing complexity. Continuing the basic principles of single-phase lattice gases, the two-phase collision operator should be kept as simple as possible, for the sake of both easy implementation and theoretical validation. At the same time it is required that parameters such as surface tension, diffusion and viscosity obtain physically relevant values. In this paper the authors present a two-dimensional two-phase model, based on a strictly local 16-bit collision operator, which incorporates a respectable surface tension relatively independent of the density.

Spohn, Herbert. Tracer diffusion in lattice gases, *J. Stat. Phys.* **59**: 1227–1239 (1990).
It has been proved that a tracer particle in a reversible lattice gas converges to Brownian motion. However, only in a few particular cases has a strictly positive self-diffusion coefficient, D, been established. Here we supply the missing piece and show that $D > 0$ in general. The exceptions are one-dimensional lattice gases with nearest neighbor jumps only, for which $D = 0$. The proof establishes a variational formula for D which could be used to obtain realistic bounds.

Squier, Richard, and Kenneth Steiglitz. Testing parallel simulators for two-dimensional lattice-gas automata, *Complex Systems* **5**:63–88 (1991).
The authors describe a test method for lattice-gas automata of the type

introduced by Frisch, Hasslacher, and Pomeau (1986). The test method consists of inserting test patterns into the initial state of the automaton and using a graphics display to detect errors. The test patterns are carefully constructed limit cycles that are disrupted by errors occurring at any level of the simulator system. The patterns can be run independently to test the system for debugging purposes, or they can be run as sub-simulations embedded in a larger lattice-gas simulation to detect faults at runtime. The authors describe the use of this method on a prototype parallel machine for lattice-gas simulations, and discuss the range of systems that can make use of this type of test method. The test patterns detect all significant one-bit errors. They include experimental results that indicate multiple-bit errors are unlikely to escape detection.

Stockman, H. W., C. T. Stockman, and C. R. Carrigan. Modeling viscous segregation in immiscible fluids using lattice-gas automata, *Nature* **34**:523 (1990).

When immiscible liquids with different viscosities are forced to flow through a channel, the more viscous liquid tends to concentrate in the center. This process influences the flow of oil–water mixtures in pipelines, the extrusion of polymers, the flow of blood in small arteries and of magmas approaching the Earth's surface during a volcanic eruption. Segregation occurs because it minimized the pressure required to maintain a given flow rate; there is still scant information, however, on the time scales and fluid configurations involved in the approach to the equilibrium state. Explicit solutions of the time-dependent Navier–Stokes equation using numerical (for example, finite-element) methods are possible only for simple interface shapes. Here the authors use an alternative approach to the study of viscous segregation, involving immiscible lattice-gas automata. Two-dimensional calculations exhibit the expected segregation for a variety of starting configurations, and for an initially homogeneous emulsion the fluid must flow 50–100 times the channel width before most of the more viscous fluid reaches the channel center. For constant flow rates, segregation occurs so as to progressively decrease the pressure.

Succi, S., A. Cancelliere, C. Chang, E. Foti, M. Gramignani, and D. Rothman. A direct computation of the permeability of three-dimensional porous media, International Conference on Numerical Methods in Groundwater Resources, Venice, 1990, *Computational Mech. Institute*, to appear.

The authors present a series of high-resolution numerical simulations of flows in porous media with the Lattice Boltzmann method. Quantitative evaluations of the medium's permeability as a function of the porosity are presented.

Succi, S., R. Benzi, and F. Higuera. The lattice Boltzmann equation: A new tool for computational fluid dynamics, *Physica D* **47**:219–230 (1991).
The authors present a series of applications which demonstrate that the lattice Boltzmann equation is an adequate computational tool to address problems spanning a wide spectrum of fluid regimes, ranging from laminar to fully turbulent flows in two and three dimensions.

Succi, S., R. Benzi, and M. Vergassola. Recent advances in the theory of the lattice Boltzmann equation, in *Proceedings Euromech Colloquium 267. Series on Advanced Mathematics for Applied Sciences*, A. S. Alves, ed. (World Scientific, Singapore, 1991), pp. 97–103.
In the recent years, a new type of fully discrete Boltzmann equation, arising from the microdynamics of Lattice Gas, i.e., a special class of cellular automata specifically designed to simulate hydrodynamic behavior, has proved to perform quite competitively for the numerical simulation of a wide variety of complex hydrodynamical phenomena. The special type of Boltzmann equation, normally referred to as the Lattice Boltzmann Equation (LBE), has in fact successfully been employed in the simulation of a wide span of hydrodynamical regimes, ranging from laminar flows in porous media to fully developed turbulent flows. In this paper, the authors present some recent developments in the theory of LBE together with a quantitative discussion on the possibility to extend LBE to the domain of two-dimensional magneto-hydrodynamics.

Succi, S., M. Vergassola, and R. Benzi. Recent advances in the theory of the lattice Boltzmann equation, *Phys. Rev. A* **43**:4521–4524 (1991).
It is shown that the lattice Boltzmann equation arising from the basic lattice-gas scheme for Navier–Stokes equations can be extended in such a way as to include the effects of a two-dimensional magnetic field. This offers the possibility of developing new computational schemes for the efficient simulation of incompressible magnetohydrodynamic flows.

Succi, S., R. Benzi, and F. Stella. A discrete kinetic scheme for the Navier–Stokes equations, ASME Meeting, Dallas, 103, Book n. G00570 (1990).

Succi, S., Foti, E., and M. Gramignani. Flow through geometrically irregular media with lattice gas automata, *Meccanica* **25**:253 (1990).
The determination of the permeability is an interesting problem of fluid dynamics of wide interdisciplinary concern. Many authors approached this subject by developing numerical models of flows through porous media at either macro-scale and micro-scale. According to the latter point of view, we present in this paper a verification of Darcy's law and a first determination of the permeability starting by the knowledge of the microstructure of

a three-dimensional random medium. The flow is here reproduced by using a particular class of cellular automata with the Boltzmann approximation.

Taylor IV, Washington, and Bruce M. Boghosian. Renormalization of lattice gas transport coefficients, Thinking Machines Corporation Technical Report, TMC-208, September 20, 1991.
A method is described for calculating corrections to the usual Chapman–Enskog analysis of lattice gases due to buildups of correlations. It is shown that renormalized transport coefficients can be calculated perturbatively by summing terms in an infinite series. A diagrammatic notation for the terms in this series is given, in analogy with the Feynman diagrams of quantum field theory. Some results for specific lattice gases are mentioned.

Tiem, Dang Hong. Exact solutions for some discrete models of the Boltzmann equation with multiple collisions, *C. R. Acad. Sci. II Paris* **313**:995–998 (1991).
A method is proposed to construct exact solutions for discrete models of the Boltzmann equation with multiple collisions. The method is applied to the case of a 10-velocity model, in which the evolution of gas depends only on triple collisions.

Toffoli, Tommaso, and Norman Margolus. Programmable matter: Concepts and realization, *Physica D* **47**:263–272 (1991).
This paper is a manifesto, a brief tutorial, and a call for experiments on *programmable matter* machines.

Toscani, G., and W. Walus. Recent results on the fractional step method in discrete kinetic theory, in *Proceedings Euromech Colloquium 267. Series on Advanced Mathematics for Applied Sciences*, A. S. Alves, ed. (World Scientific, Singapore, 1991), pp. 123–130.
The authors derive a local existence and uniqueness result for the Broadwell model in a plane box with specular reflection, by using the classical approximation method of fractional steps.

van der Hoef, M. A., M. Dijkstra, and D. Frenkel. Velocity autocorrelation function in a four-dimensional lattice gas, *Europhys. Lett.* **17**:39–43 (1992).
The authors report simulations of the velocity autocorrelation function (VACF) of a tagged particle in a *four*-dimensional lattice gas cellular automaton. The authors observe a hydrodynamic tail in the VACF, which decays as t^{-2}, in agreement with the theoretical predictions. However, in a quantitative comparison, the simulations show that mode-coupling theory underestimates the amplitude of the hydrodynamic tail by 15–60%. The artificial correlations, previously observed in the projected three-dimensional lattice gas model, are found to be absent in this truly 4D model.

van der Hoef, M. A., and D. Frenkel. Tagged particle diffusion in 3D lattice gas cellular automata, *Physica D* **47**:191–197 (1991).
The authors report simulations of tagged particle diffusion in three-dimensional lattice gas cellular automata. In particular the authors looked at the decay of the velocity autocorrelation function (VACF) using a new technique that is about a million times more efficient than the conventional techniques. For longer times the simulations clearly show the algebraic $t^{-3/2}$ tail of the VACF. The authors compare the observed long-time tail with the predictions of mode-coupling theory. In three dimensions, the amplitude of this tail is found to agree within the (small) statistical error with these predictions.

van der Hoef, M. A., and D. Frenkel. Evidence for faster-than-t^{-1} decay of the velocity autocorrelation function in a 2-D fluid, *Phys. Rev. Lett.* **66**:1591–1594 (1991).
The authors report very accurate simulations of the velocity autocorrelation function (VACF) of a tagged particle in a two-dimensional lattice gas cellular automaton. The authors observe, for the first time, that the hydrodynamic long-time tail of the VACF decays significantly faster than t^{-1}. The simulation results are compatible with the predictions of self-consistent mode-coupling theory. However, observation of a true $(t\sqrt{\ln t})^{-1}$-decay that is predicted by the latter theory as $t \to \infty$, would require simulations that are 15 orders of magnitude longer than is presently feasible.

van der Hoef, M. A., D. Frenkel, and A. J. C. Ladd. Self-diffusion of colloidal particles in a two-dimensional suspension: Are deviations from Fick's law experimentally observable? *Phys. Rev. Lett.* **67**:3459–3462 (1991).
Simulations of a colloidal particle suspended in a two-dimensional fluid are reported. The dissipative and fluctuating hydrodynamics forces acting on the particle are modeled by a lattice gas. Our results indicate that large long-time tails are present in both the translational and the rotational velocity correlation functions; these are the first observations of a rotational long-time tail. The strong translational tail leads to an observable renormalization of the diffusion coefficient; our results suggest that experimental observation of the latter effect is possible.

van der Hoef, M. A., and D. Frenkel. Long-time tails of the velocity autocorrelation function in two- and three-dimensional lattice-gas cellular automata: A test of mode-coupling theory, *Phys. Rev. A* **41**:4277–4284 (1990).
The authors report simulations of the velocity autocorrelation function

(VACF) of a tagged particle in two- and three-dimensional lattice-gas cellular automata, using a new technique that is about a million times more efficient than the conventional techniques. The simulations clearly show the algebraic $t^{-D/2}$ tail of the VACF. The authors compare the observed long-time tail with the predictions of mode-coupling theory. In three-dimensions, the amplitude of this tail is found to agree within the (small) statistical error with these predictions. In two dimensions, small but significant deviations from mode-coupling theory of up to 5% are observed.

Van Velzen, G. A. Deterministic lattice Lorentz gas: I. Chiral model, *J. Physics A* **24**:787–806 (1991).
We study diffusion by using a specific type of cellular automaton, where particles move in a random environment of scatterers. The deterministic collision rules, used in the model, give rise to certain difficulties related to non-ergodicity. The class of models, introduced by Gunn and Ortuño, also contains the model studied by Gates. Previously developed theory, including Boltzmann approximation, ring and repeated ring approximations, and effective medium approximation (EMA), is generalized for this model. The validity is further investigated using computer simulations. In the presence of reflecting scatterers EMA yields low-density results that show the *breakdown* of the Boltzmann equation, while they agree quantitatively with the low-density simulations. EMA also agrees with a phase transition that occurs for some parameter choices.

Van Velzen, G. A. Deterministic lattice Lorentz gas: II. Mirror model, *J. Phys. A* **24**:807–825 (1991).
As a model for diffusion, a lattice version of the Lorentz gas is studied, using specular collision rules. A previously developed theory, containing the molecular chaos approximation, several ring approximations and the effective medium approximation, is applied and compared with simulations. The correction to the Boltzmann equation result, resulting from the effective medium approximation, is opposite to the simulation results. This indicates that other diagrams than ring diagrams should be considered, which is peculiar if one considers the successes of the effective medium approximation for other models. This is investigated by using variants of the model. The diffusion tensor in in general non-isotropic. The corresponding features are qualitatively described by theory.

Van Velzen, G. A. Lattice Lorentz gases, Ph.D. Dissertation, University of Utrecht (1990).

Van Velzen, G. A. Lattice Lorentz gas: Kinetic theory, *J. Phys. A* **23**:4953 (1990).
Standard approximation schemes in kinetic theory are compared with the

effective medium approximation (EMA) that was developed earlier for the stochastic Lorentz gas on cubic lattices. In models with reflecting collisions the low-density results are in strong disagreement with molecular chaos and in excellent agreement with the simulation data. The present analysis identifies the diagrams that are taken into account in the different approximations. The EMA accounts in a self-consistent way for *all* nested ring diagrams.

Vergassola, M., R. Benzi, and S. Succi. On the hydrodynamic behavior of the lattice Boltzmann equation, *Europhys. Lett.* **13**:411 (1990).
The hydrodynamic behavior of the lattice Boltzmann equation in two and three dimensions is discussed. By inspecting the spectral properties of the collision operator, a natural distinction between hydrodynamic and nonhydrodynamic fields arises, which allows a clear analysis of the convergence of the model to the Navier–Stokes equations.

Vives, E., and A. Planes. Monte Carlo simulation study of a smectic–nematic-like transition in a two-dimensional lattice gas model of cylindrical particles, *Physica Scripta* **38**:75 (1991).
Monte Carlo simulation of a two-dimensional lattice gas model of orientable particles is used to study the coupling between the smectic–nematic phase transition and the orientation order parameter in Liquid Crystals. The phase diagram of the model is obtained, and the critical behavior of the smectic–nematic-like transition studied. Results can be qualitatively compared with experimental data and suggest a microscopic explanation of the continuous variation of the effective critical exponents in some Liquid Crystal mixtures. The existence of a Tricritical Point is also reproduced. Finally, results are analyzed in terms of a general Landau free energy functional [Anisimov *et al. Phys. Rev. A* **41**, 6749 (1990)] that suggests that the Tricritical Point is only apparent.

Wang, F., and E. G. D. Cohen. Diffusion in a fully occupied hexagonal lattice gas, March Meeting of the Americal Physical Society, Indianapolis, Indiana (1992).
The diffusion of a point particle on a hexagonal lattice, fully occupied by deterministic scatterers, has been studied and compared with that on a square and triangular lattice. 3000 particles on a 1024×1024 lattice with periodic scatterer boundary conditions have been used. Four cases have been considered in which the scatterers are either (left or right) mirrors or (left or right) rotators, which can or cannot flip from one orientation (left or right) to the other (right or left) upon collision. The diffusion process is in general non-Gaussian due to closed orbits, even in the flipping scatterer

cases. This in contrast to the Gaussian diffusion found for scatterers with probabilistic scattering rules.

Wells, J. T., D. R. Janecky, and B. J. Travis. A lattice gas automata model for heterogeneous chemical reactions at mineral surfaces and in pore networks, *Physica D* **47**:115–123 (1991).
A lattice gas automata (LGA) model is described which couples solute transport with chemical reactions at mineral surfaces and in pore networks. Chemical reactions and transport are integrated into a FHP-I LGA code as a module so that the approach is readily transportable to other codes. Diffusion in box calculations is compared to finite element Fickian diffusion results and provides an approach to quantifying space-time ratios of the models. Chemical reactions at solid surfaces, including precipitation/dissolution, sorption, and catalytic reaction, can be examined with the model because solute diffusion and mineral surface processes are all treated explicitly. The simplicity and flexibility of the LGA approach provides the ability to study the inter-relationship between fluid flow and chemical reactions in porous materials, at a level of complexity that has not previously been computationally possible.

Zanetti, G. Counting hydrodynamic modes in lattice gas automata models, *Physica D* **47**:30–35 (1991).
A Monte Carlo scheme for the search of extensive conserved quantities in lattice gas automata models is described. It is based on an approximation to the microscopic dynamics and it amounts to estimating the dimension of the eigenspace with eigenvalue 1 of a linear operator related to the lattice gas automata model evolution operator linearized around equilibrium distributions. The applicability of this technique is limited to models with collision rules satisfying semi-detailed balance.

Zanetti, Gianluigi. Lattice gas automata: Comparison of simulation and theory, in *Microscopic Simulations of Complex Flow*, M. Mareschal, ed. (Plenum Press, New York, 1990), pp. 47–56.
In this chapter, I will review some of the work that Leo Kadanoff, Guy McNamara and I have done on the study of the hydrodynamic behavior of Lattice Gas Automata, a technique that was recently proposed by Uriel Frisch, Brosl Hasslacher, and Yves Pomeau for the numerical solution of the incompressible Navier–Stokes equation. In our work we have been mainly concerned with testing the theoretical understanding of the LGA mode. We probed the hydrodynamical behavior of the LGA first with a gross check, based on a two-dimensional channel flow, later with a rather delicate check based on a peculiarity of two-dimensional fluids: the infrared

divergence of transport coefficients. The LGA reproduced quite accurately the parabolic momentum density profile expected in the simulation of the channel flow. However, in the delicate check there is a discrepancy of about 30% between the simulation results and theory. We have been able to explain this discrepancy, but in doing so we have discovered that the hydrodynamic behavior of this simple lattice gas automata is actually more complicated than the behavior of simple fluids.

Ziff, Robert M., X. P. Kong, and E. G. D. Cohen. Lorentz lattice-gas and kinetic-walk model, *Phys. Rev. A* **44**:2410–2428 (1991).
The Ruijgrok–Cohen (RC) mirror model [*Phys. Lett. A* **133**, 415 (1988)] of a Lorentz lattice gas, in which particles are reflected by left and right diagonally oriented mirrors randomly placed on the sites of a square lattice, is further investigated. Extensive computer simulations of individual trajectories up to 2^{24} steps in length, on a lattice of 65536×65536 sites, are carried out. This model generates particle trajectories that are related to a variety of kinetic growth and "smart," (nontrapping) walks, and provides a kinetic interpretation of them. When all sites are covered with mirrors of both orientations with equal probability, the trajectories are equivalent to smart kinetic walks that effectively generate the hulls of bond percolation clusters at criticality. For this case, 10^6 trajectories were generated, yielding with unprecedented accuracy an orbit size-distribution exponent of $\tau = 2.1423 \pm 0.0003$ and a fractal dimension of $d_F = 1.75047 \pm 0.00024$ (without correcting for finite-size effects), compared with theoretical predictions of $\frac{15}{7} = 2.142857...$ and $\frac{7}{4}$, respectively. Then the total concentration of mirrors C is less than unity, so that the trajectories can cross, the size distribution of the closed orbits does not follow a power law, but appears to be described by a logarithmic function. This function implies that all trajectories eventually close. The geometry of the trajectories does not show clear self-similar or fractal behavior in that the dependence of the mean-square displacement upon the time also appears to follow a logarithmic function. These trajectories are related to the growing self-avoiding trail (GSAT) introduced by Lyklema [*J. Phys. A* **18**, L617 (1985)], and the present work supports the conjecture of Bradley [*Physical Review A* **41**, 914 (1990)] that the GSAT (The RC model with $C = \frac{2}{3}$) is not at a critical point. It is observed that when $C < 1$, the trajectories behave asymptotically like an unrestricted random walk, and so for comparison the RC model in the random walk or Boltzmann approximation (BA) is also studied. In the BA, the size distribution of returning trajectories and the geometric properties of open trajectories are investigated; the time dependence of the mean-square displacement is derived explicitly and is shown to exhibit an Ornstein–Uhlenbeck type of behavior.

The following are solid-state or Ising model-related papers which also describe themselves as "lattice-gas" oriented. They often use Monte Carlo methods in their descriptions. The following papers are only a small sample to indicate their areas of interest. Including all such papers would have tripled the length of this bibliography.

Andersen, Jorgen Vitting, Henrik Jeldtoft Jensen, and Ole G. Mouritsen. Crossover in the power spectrum of a driven diffusive lattice-gas model, *Phys. Rev. B* **44**:439 (1991).
A driven diffusive lattice-gas model with stochastic dynamics is used to study, via a Monte Carlo simulation, the fluctuation in the particle density and the lifetime of the particles in the system. The scaling properties of the power spectrum and the lifetime distribution function exhibit a crossover from $1/f^{\beta}$ to $1/f^2$-behavior, with $\beta = 1.5$, when the drive is sufficiently strong to induce a characteristic time scale. We argue that the scaling behavior with $\beta = 1.5$ is governed by the stochastic nature of the dynamics, whereas deterministic dynamics leads to $\beta = 1$.

Bozek, P., Z. Burda, and J. Jurkiewicz. Intermittency and clustering in the 1D lattice gas model, *Phys. Lett. B* **265**:133 (1991).

Burlatsky, S. F., G. S. Oshanin, and M. M. Elyashevich. Diffusion-controlled deposition of a dense lattice gas, *Phys. Lett. A* **151**:538 (1990).
The authors study the diffusion-controlled deposition of a two-dimensional hard-core lattice gas in systems where the temperature is quenched to zero not uniformly in the volume, but on the boundary only. The authors show that the patterns grown are inhomogeneous dense packing of tree-like clusters, which do not penetrate into each other. The authors present the simulation results that document the occurrence of fluctuation-induced forms of cluster-cluster screening, resulting in a decrease of the *number of clusters*, N, with the growth of the pattern's height h, $N(h) \approx h^{-1/2}$.

Jackle, J., K. Frobose, and D. Knodler. Size dependence of self-diffusion in the hard-square lattice gas, *J. Stat. Phys.* **63**:249 (1991).
A striking size dependence of the mean-square displacement of diffusing particles in the two-dimensional lattice gas of hard squares has been observed by Monte Carlo simulation. It is shown that the size effect is due to the formation of a stable cage structure in small lattices when the particle concentration is high. The formation of cages is governed by a new type of percolation problem related to bootstrap percolation.

Meakin, Paul, and M. Muthukumar. The effects of attractive and repulsive interaction on two-dimensional reaction-limited aggregation, *J. Chem. Phys.* **91**:3212 (1989).
The effects of both attractive and repulsive interactions on reaction-limited

cluster-cluster aggregation have been explored using a two-dimensional polydisperse off-lattice model. Interactions with a magnitude on the order kT (k is the Boltzmann constant and T is temperature) have an important effect in both the aggregate structure and the kinetics of aggregation.

Patrykiejew, A., and P. Borowski. A two-dimensional Lennard-Jones lattice gas, *Thin Solid Films* **195**:367 (1991).

Percus, J. K. Entropy of a one-dimensional mixed lattice gas, *J. Stat. Phys.* **60**:221 (1990).

Percus, J. K., and Guihua Zhang. One-dimensional lattice gas with second-neighbor interaction, *Phys. Rev. A* **42**:731 (1990).

Protasov, I. D. Equation of state of a lattice gas, *Sov. Phys. Doklady* **35**:791 (1990).
Ideal models of matter (perfect gas, lattice gas, etc.) are useful in theoretical physics since they enable us to obtain relatively simply the thermodynamic functions of state of a medium which in some sense is ideal; they can be used under well-defined physical conditions and taking into account the correct procedure for identifying a real medium to prognosticate thermodynamic characteristics and also to construct more complicated models of physical media and the processes occurring in them.