ABSTRACTS FOR THE FIELDS INSTITUTE FOR RESEARCH IN MATHEMATICAL SCIENCES AND NATO ADVANCED RESEARCH WORKSHOP PROGRAM

PATTERN FORMATION and LATTICE-GAS AUTOMATA

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1. C. Appert, Université Pierre et Marie Curie, France
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23. S.R.S. Varadhan, Courant Institute, USA
24. X.-G. Wu, University of Toronto, Canada
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35. J. Yepez, Phillips Laboratory, USA  
36. C. Yu, University of Tokyo, Japan
ABSTRACTS OF INVITED TALKS

Large Liquid-Gas Models on 2D and 3D Lattices
Cécile Appert and Stéphane Zaleski
Laboratoire de Modélisation en Mécanique, CNRS,
Université Pierre et Marie Curie, Tour 66,
4 Place Jussieu, 75252 Paris Cedex 05, France

Liquid gas models on a lattice are derived from lattice gas cellular automata by adding interactions at a distance. These interactions allow to create a separation of phases. An interface between a liquid phase and a gas phase is created spontaneously. The model is found to obey the Boltzmann molecular chaos assumptions quite well. The surface tension and the viscosity may be predicted using this assumption and an expansion in large interaction distance. The origin of the non-Galilean factor will also be discussed. Extensions to three dimensions were performed recently. Example of applications are the formation of soap froth and flow in porous media.

Correlations and Renormalization in Lattice Gas Automata
B. Boghosian
Thinking Machines Corporation
245 First Street
Cambridge, MA 02142–1214, USA

A method is described for calculating corrections to the usual Chapman-Enskog analysis of lattice gases due to the buildup of correlations. For lattice gases satisfying semi-detailed balance, and analyzed in the diffusion limit ($\Delta t \sim (\Delta x)^2$), it is shown that exact renormalized transport coefficients can be calculated perturbatively by summing a diagrammatic series. Closed-form expressions are given for the vertices in these diagrams. It is shown that subsets of these diagrams can be easily identified that correspond to the kinetic ring approximation, or to any truncation of the BBGKY hierarchy. This method is applied to several example lattice gases, and results are shown to be in agreement with numerical experiments.
Fluctuation Correlations in Lattice-Gas Automata  
Jean Pierre Boon  
Physique Non-Lineare et Mécanique Statistique  
Université Libre Bruxelles  
1050 Bruxelles, Belgium

Some aspects of the Statistical Mechanics of Lattice-Gas Automata will be reviewed with emphasis on density fluctuation correlations. A comparative analysis of theoretical predictions and simulation results will be presented.

Lattice Boltzmann Method and its Application in Computational Biology  
Shiyi Chen  
Theoretical Division and Center for Nonlinear Studies  
Los Alamos National Laboratory  
Los Alamos, NM 87545, USA

In this talk, we will present our recent results of the application of lattice Boltzmann method in biological systems, including simulation of cytoskeleton and polymeric fluids.

Diffusion, Propagation and Pattern Formulation in Lorentz Lattice Gases  
E. G. D. Cohen and F. Wang  
The Rockefeller University,  
New York, NY 10021, USA

In a Lorentz lattice gas point particles move, without mutual interactions, on the bonds of a lattice, whose sites are partly or fully occupied by scatterers. For the strictly deterministic scattering rules for the particles by the scatterers considered here, the behavior of the particles differs fundamentally from that for probabilistic scattering rules. Various types of diffusive behavior, as well as propagation and pattern formulation have been observed in computer simulations, depending on the structure of the lattice, the nature of the scatterers and their distribution over the lattice. Neither probability theory nor kinetic theory can account for these phenomena, but a different theoretical approach, recently initiated by Bunimovich and Troubetskoy has lead to a number of theorems on the behavior of the particles on the lattice.
Polymerization through Heterogeneous Catalysis: a Reactive Lattice-Gas Automaton Approach

D. Dab
Physique Non-Lineare et Mécanique Statistique
Université Libre Bruxelles
1050 Bruxelles, Belgium

We justify the need for a simple microscopic approach to polymerization through heterogeneous catalysis and we construct a reactive lattice-gas automaton model which is used to discuss the problem of the broad molecular-weight distribution observed in real experiments.

Glauber Evolution with Kac Potentials

A. De Masi
Dipartimento di Matematica
Università dell'Aquila,
67100 l’Aquila, Italy

In a typical quenching experiment there are different regimes with their own space-time scale and their characteristic phenomena. The early stage is when the phases develop emerging from the initial unstable state. Clusters of the thermodynamically stable phases appear, still relatively small, macroscopically, but large enough microscopically, to allow for an accurate statistical description. In the next stage the clusters move and this is called the interface dynamics regime.

I study these phenomena in the Glauber spin flip dynamics with $\pm 1$ valued spins interacting via a Kac potential. The temperature is fixed below the critical value and the initial measure is product with zero average corresponding to a value of the magnetization which is thermodynamically unstable. At times which grow logarithmically in the scaled length of the Kac interaction, the early stage of the spinodal decomposition is observed. We characterize the typical spin configurations both during the separation and at the time when the clusters of the two phases appear. This analysis is strictly related to the study of the solution of the non local evolution equation describing the macroscopic behavior of the model. The successive motion of the interfaces is also analized showing that the late stage of the spinodal decomposition in this isotropic system with non conserved order parameter, is described by a motion by mean curvature.
Future Computers and Lattice Methods; Multiphase Flows Through Porous Media

G. D. Doolen
Center for Nonlinear Studies and Theoretical Division Los Alamos National Laboratory
Los Alamos, NM 87545, USA

Recent developments in electronic devices have shown that lattice gas emulations could possibly be executed on extremely fast components, with the possibility that orders of magnitude increase in speed might be possible. A summary of developments to date will be given along with some description of progress made in self-assembling computers. Also 3D lattice Boltzmann calculations of high-resolution multiphase flows through porous media (10 micron tomographic pore scale data provided by Mobil Oil, Inc.) will be described and videos shown.

Metastability and Pattern Formation in Biased Lattice Gases

Matthieu H. Ernst
Institute for Theoretical Physics
University of Utrecht
3508 TA Utrecht, The Netherlands

Self organization or dynamic phase transitions occur in computer simulations of a lattice gas with strictly local, but asymmetric collision dynamics, conserving mass, momentum and lattice symmetries. A spatially uniform initial state is unstable. At the onset of instability long wavelength modes drive the system into a state with long range order. Different domains are not only characterized by a scalar order parameter (mass density), but also by one with vector character (momentum density). The structure factors and spatial correlation functions for the different order parameters are measured and analyzed in terms of scaling laws. The state with long range order is highly organized into moving stable spatial patterns of triangles and parallel strips of macroscopic size. The onset of instability as well as the structure of domains and interfaces is well described by mean field theory. The emphasis at this stage concern the existence and possible structure and spatial correlations of stationary states or limit cycles in microscopic models that violate the detailed balance conditions.
Lattice BGK Models for Miscible Fluid Flow: Experiment and Simulations
E. G. Flekkøy*, U. Oxaal**, J. Feder**, T. Jossang**

* Center for Advanced Study
at The Norwegian Academy of Science and Letters
P.O.Box. 7606 Skillebekk
0205 Oslo, Norway

*Departament of Physica
University of Oslo
Box 1048 Blindern
0316 Oslo 3, Norway

We present a comparison between Lattice BGK simulations and a hydrodynamic dispersion experiment performed in a Hele–Shaw with simple internal geometry. The aim of this work is to verify the models’ to reproduce quantitatively the experimental results as well to provide a tool for the extension of these results. Comparison of the dispersed concentration profiles provides a test of both the hydrodynamic and the diffusive behavior of the model, and preliminary results show good agreement between simulations and experiment.

The two dimensional BGK model simulates, in a simplified way, the full three dimensional features of the experiment flow. Although the experiment is performed at a very low Reynolds number, small effect of nonlinearity is observed. For steady state flow the model contains a parameter that allows tuning of the Reynolds number independently of the flow velocity, viscosity and system size. This is used to study this effect over a wider range of parameters than what is experimentally accessible.

Lattice Gases and New Emergent Complexity in Biochemical Systems
Brosl Hasslacher
Complex Systems Group Theoretical Division and
Center for Nonlinear Studies
Los Alamos National Laboratory
Los Alamos, New Mexico 87545, USA

Recently, there have been several remarkable developments in new origins of complexity at the cellular and sub-cellular levels, which are only accessible at present using large parallel machines of the CM class. The main biochemical pathway under study is the glycolytic pathway in the Sel’kov approximation, which is known to be reliable in laboratory scale glycolytic reactions. We are using reactive lattice gases, which capture noise effects correctly, to study diffusion driven instabilities in these reaction-diffusion systems in several regimes.

The first is the pure Turing region where we observe classic static Turing global symmetry breaking at the 30 - 500 nanometer scale in ATP concentration, contrary to previous rough estimates.

The second is the Turing-Hopf region where we see a remarkable range of dynamic ATP concentration behavior, which so far is analytically unexplored.
The third is in the same regimes, but now using strongly perturbed initial conditions which cause the system to ring in a nonlinear way.

The latter excites a remarkable range of complex spatial dynamics that resembles the actual structures seen in biology, including cell division and growth of cell walls. This appears to be a new route to chaos. We feel this is directly relevant at least to the organization and growth of a large variety of ATP engines, including tubulin and microtubule dynamics and protein dynamics in general.

It may also shed some light on their self-assembly. Similar structures have recently been seen experimentally, in more limited regimes in other systems, by both the Texas group under Swinney and the Bordeaux group under DeKepper. It seems that there are no computational tools of similar scope available to study these effects. Their discovery throws into question nearly half century’s assumptions about biochemical dynamics at the sub-micron scale.

**Vortex Street and Lévy Walk**

**F. Hayot**
Department of Physics
Ohio State University
Columbus Ohio 43210, USA

A vortex street—the so-called von Karman street—is generated in flow around an infinite cylinder at sufficiently high Reynolds number. The vortex shedding by the cylinder occurs at a well defined frequency, and the vortices themselves have a spatial extent characterized by cylinder size. Lévy walks correspond to momentum exchanges over many scales in the flow enveloping the cylinder. Their intensity and their maximum size model the presence of some characteristic turbulence in the incoming flow. One is interested in how this turbulence affects the vortex street. The Lévy walk algorithm of lattice gas hydrodynamics provides a model where the issues of how the scales of momentum exchanges interfere with the coherent structure of the vortex street can be investigated. I will present a number of results and compare them with experiment.

**Lattice Gases without Semi-Detailed Balance**

**M. Henon**
CNRS, Observatoire de Nice,
BP 229, 06304 Nice Cedex 4, France

Is it all right to use lattice gas models without semi-detailed balance in numerical simulations of fluids? What is going on when we do that, and what are the consequences? In particular, why is the observed viscosity systematically larger than the theoretical value computed under the Boltzmann approximation? In this talk I will describe a few experiments provoked by these questions.

1. Microscopic correlations have been measured for several variants of the FCHC 24-velocity lattice gas. They include correlations between input velocities; between output velocities; between input and output velocities; between nodes; and between time steps.
Some observed features, but not all, can be explained as consequences of the criteria used to build the collision tables.

2. Measurements were also made of the components of the second-order momentum, which plays a crucial role in connection with the viscosity.

3. These measurements, taken together, lead to an explanation for the fact that the observed viscosity is larger than the theoretical Boltzmann value. An attempt was made to use this explanation to build a better FCHC collision table; unfortunately, only a marginal improvement is obtained.

4. When semi-detailed balance is violated, the phase space accessible to the system as a whole contracts with time, until eventually a stable subset is reached. This might be relevant to the observed behavior of the models. In particular it would be of interest to estimate the time scale of the contraction, and the size of the final subset. A direct numerical attack seems impossible in the FCHC case because the phase space is too huge. Therefore experiments were made with a much simpler lattice, with one dimension and two or three velocities (in progress at the time of this writing).

Exact Solutions for the Lattice Boltzmann Equation: Boundaries and Interfaces
D. d’Humières
Laboratoire de Physique Statistique
24 Rue Lhomond
75231 Paris, Cedex 05, France

Relaxation Lattice Boltzmann Equation was proposed by Higuera [1] as an improvement of Lattice Gas Models with respect to noise and ease of implementation for the 3-D models. It turns out that this scheme has exact solutions for simple flows, like Couette or Poiseuille ones, both for simple fluid model and for immiscible ones [2]. These exact solutions will be presented along with their use for a precise characterization of boundary conditions: walls, in and out flow conditions and interfaces between two fluids.

[1] F. Higuera and J. Jimenez, “Boltzmann Approach to Lattice Gas Simulations”, Europhys. Lett. 9, 663 (1989).
[2] A.K. Gustensen, D.H. Rothman, S. Zaleski, and G. Zanetti, “Lattice Boltzmann model of immiscible fluids”, Phys. Rev. A43, 107 (1991). A.K. Gustensen and D.H. Rothman, “Microscopic Modeling of Immiscible Fluids in Three Dimensions by the Lattice Boltzmann Method”, Europhys. Lett. 18, 157 (1992).
CAM-8: A Computer Architecture Based on Cellular Automata

N. Margolus
Laboratory for Computer Science
Massachusetts Institute of Technology
Cambridge, MA 02139, USA

CAM-8 is an indefinitely scalable multiprocessor optimized for spatially fine-grained, discrete modeling of physical systems—such as lattice-gas simulations of fluid flows. With an amount and kind of hardware comparable to that in an inexpensive workstation (64 Megabytes of conventional DRAM and 2 Megabytes of cache-grade SRAM, all running with a 25 MHz clock) our small-scale prototype already performs a wide range of such simulations at speeds comparable to the best numbers published for any commercial machine. Machines orders of magnitude bigger and proportionately faster can be built immediately, using the existing (working) chips. This kind of computing power has never before been available for spatially fine-grained modeling: CAM-8 makes a new band of the computational spectrum effectively accessible.

The Discrete Boltzmann Equation for Gases with Bi-Molecular or Dissociation-Recombination Reactions

Roberto Monaco
Department of Mathematics
University of Genoa
Via L. B. Alberti 4 - 16132 Genova-Italy

In recent years, new interest has been devoted to real gas effects due chemical reactions. In fact, as well documented by the Proceedings book of an IUTAM Symposium [1], in the near future, several space missions are foreseen in the atmosphere of celestial bodies of our planetary system where chemical reactions play a major role. In this physical situation, problems including combustion [2], catalytic gas-surface interactions [3], and onset of shock-waves and of detonation waves [4] must be investigated both at the macroscopic and the microscopic level.

A physical mathematical tool which seems to be promising, for the representation at a microscopic level of a chemically reacting gas mixture, is the Discrete Boltzmann Equation (DBE), see Chap. 6 of book [5].

This paper has the aim of proposing two kinetic models of the DBE, the first representing gases undergoing bi-molecular reactions, the second representing gases with dissociation-recombination reactions.

The first model considers a mixture of four gases undergoing elastic collisions and reactions of the type

$$A + B \rightleftharpoons C + D.$$  

The second is related to reactions for a diatomic gas $A_2$, i.e.

$$A_2 + M \rightleftharpoons A + A^* + M$$

and considers binary and triple elastic collisions as well. In the second equation, $A$ are atoms and $A^*$ atoms at a higher energy level. $M$ is a catalyzer which can be either a molecule $A_2$, either an atom $A$ or either a high energetic atom $A^*$. 
For the first model we choose a Broadwell-type discretization of velocity, i.e.

\[ \mathbf{v}^M_i = \mu_M c \mathbf{e}_i, \quad i = 1, \ldots, 6, \quad M = A, B, C, D, \]

\( \mu_M \) being the mass ratios \( m_M/m_A; c \) is a reference speed and \( \mathbf{e}_i \) are unit vectors oriented towards the positive and negative directions of the axes of a spatial orthogonal frame.

The second model is derived in the plane. In detail, we consider a square centered in the origin of an orthogonal frame. Then the velocities of atoms \( A \) are directed in the positive and negative directions of the \( x \)- and \( y \)-axes. Molecules have the same velocities as atoms but with a smaller speed. Atoms \( A^* \) finally have velocities in the direction of the four vertices of the square. In symbols

\[ A : \mathbf{v}_i = c \mathbf{e}_i, \quad i = 1, \ldots, 4, \quad \mathbf{e}_i = \{i, j, -i, -j\} \]

\[ A_2 : \mathbf{v}_i = \mu c \mathbf{e}_i, \quad \mu = 1/2 m_A \]

\[ A^* : \mathbf{v}^*_i = c i_i, \quad i_i = \{\sqrt{2}(i + j), \sqrt{2}(-i + j), \sqrt{2}(-i - j), \sqrt{2}(i - j)\}, \]

where \( m_A \) is the mass of the atom and \( c \) again a reference speed. For both models, we write the kinetic equations, following the hypothesis:

1) Elastic and chemical interactions are characterized by different collision frequencies.

2) Each collision preserves mass, momentum and energy (including chemical link energy).

In the present paper, starting from this point, we derive for both models

- the space of collisional invariants and the conservation equations
- the H-theorems, the thermodynamical equilibrium conditions and the mass-action laws
- the Euler equations.

Moreover for the first model we obtain

- the Navier-Stokes equations and the transport coefficients.

Finally for the second model we study by numerical simulations

- the effects of the dissociation rate on the Riemann problem for the shock-waves onset.

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2. Recent Advances in Combustion Modeling, Ed. B. Larrouytrou, World Sci. Pub., Singapore, London 1991.
3. C. Bruno, in Fluid Dynamical Aspects of Combustion Theory, Eds. M. Onofri and A. Tesei, Pitman Series in Math., Longman Sci. and Tech., J. Wiley, New York, 1992, p. 329.
4. A. K. Kapila, ibidem, p. 143
5. R. Monaco and L. Preziosi, Fluid Dynamic Applications of the Discrete Boltzmann Equation, World Sci. Pub., Singapore, London, 1991.

Collision Rules for Two-Dimensional Hydrodynamics

Alain Noullez
Mech. & Aerospace Eng. Dept.
Room D-414 E-Quad, Olden Street,
Princeton University
Princeton, NJ-08544, U.S.A.

I investigate the design of optimized collision rules for the 2-D FHP lattice gas model for minimal viscosity. It is shown that for these models, the optimization reduces to a
geometrical matching problem whose solution can be obtained explicitly for any number of static particles. This construction is used to obtain models which are more efficient than the FCHC model for two-dimensional hydrodynamics. The effect of relaxing the constraint of semi-detailed balance and its effect on the equilibrium properties of these models is also investigated.

Lattice Boltzmann Simulations of Pattern Formation Reaction-Diffusion Systems
S. Ponce-Dawson
Center for Nonlinear Studies and Theoretical Division
Los Alamos National Laboratory
Los Alamos, NM 87545, USA

I will describe a lattice Boltzmann model for reaction-diffusion equations that has been developed recently [1]. In particular, I will discuss the ability of the scheme to simulate the formation of patterns in these systems. I will analyze the appearance of these patterns due to the Turing instability in cases with and without convection of the reactants, the differential flow induced instability and the interaction among them.

1. S. Ponce-Dawson, S. Chen, and G. Doolen, J. Chem. Phys. 98, 1514 (1993)

Critical Fluctuations in Spin Systems
Errico Presutti
Dipartimento di Matematica
II Università degli Studi di Roma
Via Fontanile di Carcaricola
00133 Roma, Italy

I consider an Ising spin system on the lattice $\mathbb{Z}^d$ with ferromagnetic interactions given by a Kac potential. The problem that I want to discuss concerns the structure of the macroscopic fluctuations of the magnetization at the critical temperature, in the scaling limit when the range of the Kac potential becomes infinite. In particular the question is when the limiting process is non Gaussian and, in that case, a control of the ultra-violet divergencies in the discrete approximation.

Gibbsian equilibrium and non equilibrium Glauber spin flip dynamics are considered. In $d=1$, it is proven that, on a given space time scaling, the fluctuations process, suitably renormalized, converges to a non linear Ginzburg Landau equation with noise. In particular therefore we have that a discrete model for the stochastic quantization of the anharmonic oscillator is the Ising Glauber dynamics with Kac potentials at the critical temperature. The convergence result is derived by comparison of the true process with another spin flip evolution, known as the voter model. It is shown that while the voter model converges to the Gaussian process given by the linear Ginzburg Landau equation with noise, the density (Radon Nykodim derivative) with respect to the voter model converges to the density of the non linear Ginzburg Landau equation with respect to the linear one.

In $d=2$, I consider the equilibrium fluctuations and prove the following. If the inverse critical temperature, $\beta = 1$, is approached from below (with suitable speed) then the
limiting process is Gaussian with an extra mass related to the Wick regularization term. This leads to the conjecture that the non linear evolution can be actually derived by approaching the critical temperature with some different speeds. The dynamical aspects of this procedure are also discussed.

**Lattice Gas Transport in Porous Media**

R. Rechtman* A. Salcido**

* Depto. de Física, Facultad de Ciencias, UNAM, Apdo. Postal 70-542
  04510, M‘exico D.F., M‘exico

** Instituto de Investigaciones Eléctricas,
  Apdo. Postal. 475
  6200, Cuernavaca Mor., Mexico

A nine velocities lattice gas is used for computer simulations of 2-d flows through random porous media. We study self diffusion, the dependence of the diffusion coefficient on temperature and the rate flow.

**Surface Tension and Immiscible Lattice Gases**

Daniel H. Rothman

Laboratoire de Physique Statistique
Ecole Normale Supérieure
24 rue Lhomond
75005 Paris, France

The talk begins with a review of immiscible lattice-gas models and related lattice-Boltzmann models of immiscible fluids. Recent applications are briefly reviewed, with some emphasis on the problem of multiphase flow through porous media. I then describe a theoretical calculation, based on a Boltzmann approximation, of the surface tension in immiscible lattice-gas models. Among other results, the calculation shows a phase transition from a mixed state to a phase-separated state via the existence of a non-zero surface tension above a critical particle density $d_c \approx 0.2$. The accord between the theoretical predictions and empirical measurements of the surface tension are qualitatively, but not quantitatively, good. Errors are due to the neglect of correlations, which appear to strongly influence the magnitude of the surface tension at high particle densities.
Two and Three-Dimensional Simulations of Rayleigh-Bénard Turbulence with Lattice Boltzmann Method

S. Succi*, F. Massaioli**, R. Benzi**, R. Tripiccione***
* IBM European Center for Scientific and Engineering Computing
  00141 Roma, Italy
** Physics Department, University of Roma,
  Via Ricerca Scientifica
  00133 Roma, Italy
*** INFN Sezione di Pisa,
  Pisa, Italy

Numerical simulations of Rayleigh-Bénard Convection in two and three dimensions using the Lattice Boltzmann method are presented.

In particular, a number of new highlights related to the onset of soft-to-hard turbulence transition, probability distribution functions and scaling laws in thermal turbulence will be discussed.

Asymmetric Mean Zero Random Walk with Exclusion: Self Diffusion

S.R.S. Varadhan
Courant Institute, New York University
251, Mercer Street,
New York, NY 10012, USA

We study the motion of a tagged particle in equilibrium in the case of an asymmetric mean zero random walk with exclusion.
We establish convergence to Brownian motion under the usual diffusive scaling of space and time. The non-reversibility of the model causes problems and the usual methods have to be modified in order to establish the result.

Reactive Lattice-Gas Automata and Chemical Chaos

Xiao-Guang Wu
Chemical Physics Theory Group
Department of Chemistry
University of Toronto,
Toronto M5S 1A1, Canada

An overview of the methods used to construct lattice-gas cellular automata for multi-component chemically reacting systems will be given. As an example of the application and utility of this method, a mesoscopic model of the Willamowski-Rössler reaction, a three-variable system whose mean-field rate law gives rise to a strange attractor, will be constructed. The effects of fluctuations on the dynamics in the regime where “deterministic” chaos exists will be studied and the validity of the mean-field description will be examined.
A New Numerical Model of Non-Newtonian Fluids
Einat Aharonov and Daniel H. Rothman
Department of Earth, Atmospheric, and Planetary Sciences
Massachusetts Institute of Technology
Cambridge, MA 02139 USA

We introduce a new numerical model of non-Newtonian fluids based on an idealized microscopic kinetic theory. Specifically, we simulate a Boltzmann equation in which the collision dynamics are dependent on the local instantaneous strain. We use the new model to study flow through porous media, a problem that has applications in the flow of molten magma through the mantle and flow of water and contaminants through soil, and find that flux is related to force by a simple scaling law.

Lattice-Boltzmann Methods for Simulating Semi-Classical Transport Phenomena in Semiconductors
M. G. Ancona
Center for Nonlinear Studies, MS-B258
Los Alamos National Laboratory
Los Alamos, NM 87545
ancona@goshawk.lanl.gov

We discuss two different lattice-Boltzmann schemes for solving macroscopic PDEs describing semi-classical electron transport phenomena in semiconductor devices. The first scheme solves the simple yet widely-used equations of the diffusion-drift transport description. In this we include both electron and hole transport with realistic mobility models for both carrier types. The second scheme supplements the first by including effects of electron inertia, an inclusion which is important for accurate simulation of high-frequency devices. For both of these schemes we solve the coupled electrostatics problem using a lattice-Boltzmann-based relaxation procedure thereby maintaining an overall consistency of method. The poster will describe each of these schemes in some detail, give evaluations of them on numerical grounds and present results pertaining to silicon and silicon-germanium field-effect transistors obtained using them on a massively-parallel computer (CM-200/CM-5).
In this contribution, we present our lattice-Boltzmann simulations of convective flow. Our method is suited to two- and three-dimensional calculations. We use the lattice geometry presented in reference [4]. Our treatment of convective flow in the Boussinesq approximation relies on the analogy between mass and heat transport. We have already used the same principle in corresponding lattice-gas simulations, cf. references [1] and [2]. The collision term in the lattice-Boltzmann equation is represented by a two-relaxation-times model, corresponding to the two transport coefficients in the macroscopic equations. To incorporate a buoyancy force, a slight perturbation is added. We can choose the relaxation times in the domain of the known stability limits, i.e. the transport coefficients must remain positive.

Right from the beginning, we have implemented our lattice-Boltzmann model on a parallel computer with SIMD architecture. The machine, a MasPar Mp 1216, possesses a data parallel unit consisting of 16384 processor elements (PE), arranged in an array of size 128 x 128. Each PE is endowed with 16 kByte local memory. The programming has been done using the MasPar implementation of the FORTRAN 90 language. For the performance of the code, it is of importance that the communication between the PEs is done by the fast “xnet”-mechanism of the machine, which connects eight nearest neighbors to each processor.

As an application, we want to present our first simulations of thermal turbulence in Rayleigh-Bénard convection. To verify the lattice-Boltzmann algorithm in this regime, we oriented our work to the simulations presented in reference [5] (see also [7]). So the calculations are performed for a convection cell of unit aspect ratio. The Prandtl number has a value of 7 and the Rayleigh number varies between $10^5$ and $10^7$. Also in accordance with experimental findings (see references [3] and [8]), we observe waves and plumes which develop from the thermal boundary layer. Currently, closer analysis of the simulation data is in progress. Here, we will use methods of wavelet analysis, in the spirit of reference [6].

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Pattern Formation Simulation of Certain Chemical Reactions
Ayse Zehra Aroguz\(^1\) and Adnan Taymaz\(^2\)

\(^1\)Chemistry Department, Engineering Faculty, Avcilar Campus
\(^2\)Physics Department, Science Faculty, Vezneciler Campus
Istanbul University, 34459 Istanbul, Turkey

The computer simulation technique of molecular dynamics is briefly reviewed, which involves simulation of chemical reaction function of molecules on a computer from a few hundred small molecules such as \(H_2O\) or \(N_2\) over a few picoseconds to larger macro-molecules. The aim of this presentation is two fold; first to introduce a mathematical procedure which enhances visual separation of individual band of a molecule, second to deal with the investigation of certain molecular patterns of practical interest at atomic level. The validity of reaction function simulation has been dealt by comparison with experimental results.

A Discrete Kinetic Model with Chemical Reactions of Type \(A + A \rightarrow B\)
Ida Bonzani\(^1\) and M. Antonietta Cimaschi\(^2\)

\(^1\)Department of Mathematics, Politecnico di Torino
\(^2\)Department of Mathematics, University of Genova

Discrete kinetic theory for gases undergoing to chemical reactions have been introduced in [1]. As known gas mixtures with bi-molecular dissociation and recombination reactions are considered both in aerospatial engineering [2] and combustion theory [3]. The complete Boltzmann equation extended to chemically reacting gases leads to a complicated mathematical structure in terms of integro-differential equations. Discrete models seems to be more convenient in view of fluid dynamic applications and particularly in cellular automata research.

In the present paper, we consider a binary gas mixture, undergoing to the following chemical reaction: \(A + A \rightarrow B\)

Each gas species may experience binary elastic collisions too, between particles of the same species or opposite species; both chemical and elastic interactions preserve mass and momentum.

The set of admissible velocities for the gas particles is given by the following sixteen planar vectors
\[v_{2k-1}^A = ce_k, \quad (k = 1, \ldots, 4)\]
\[ v_{2k}^A = v_{2k-1}^A + v_{2k+1}^A \]
\[ v_i^B = 2v_i^A, \quad (i = 1, \ldots, 8) \]
where \( \mathbf{e}_k = \{i, j, -i, -j\} \) are vectors in the fixed frame \((O, i, j)\) and \(c\) is a reference speed.

If the number densities related to each velocity are
\[ N_i^A = N_i^A(t, x), \]
\[ N_i^B = N_i^B(t, x), \quad x \in \mathbb{R}^2, \]
the resulting kinetic equations are expressed in the form
\[
\frac{\partial N_i^A}{\partial t} + v_i^A \cdot \nabla x N_i^A = J_i^A(N^A, N^B) - R_i^A(N^A) \\
\frac{\partial N_i^B}{\partial t} + v_i^B \cdot \nabla x N_i^B = J_i^B(N^A, N^B) + R_i^B(N^A)
\]
where the terms \(J_i\) are due to elastic collisions and \(R_i\) to chemical reactions.

Mathematical properties of the model and physical implications are then considered in the paper, together with some numerical simulations where classic flows in bounded and unbounded domains are proposed and visualized.

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Towards Analyzing Complex Swarming Patterns in Biological Systems with the Help of Lattice-Gas Cellular Automata

Andreas Deutsch
Biologie
University of Bonn

Cellular automaton models have been successfully applied to biological phenomena, in particular to the formation of morphogenetic patterns [2,3,7]. Nevertheless, an important problem of cellular automata lies in their limiting behavior, i.e. the consistency of the discrete automaton formulation with continuous models written in the language of partial differential equations. From lattice-gas theory many examples are known in which this problem has been solved [4]. While the core of a (physical) lattice gas consists of rotation, propagation and collision operators mimicking the dynamics of ‘elementary particles’, chemical dynamics (e.g. of reaction-diffusion type) can be modeled by introducing additional ‘reactive’ operators [6].

Here, we address the problem of swarming behavior in biological systems. Swarming phenomena are not limited to organisms but may also occur on a cellular level. In any case, certain interactions between cells or organisms are responsible for the origin of typical swarming patterns. For example, certain salamander larvae exhibit horizontal and vertical stripe patterns of pigment cells which arise from migration, i.e. swarming of embryonic cells within the fibrous network given by the extracellular matrix [5].

A biological ‘lattice-gas’ cellular automaton is developed that is based on a piecewise straight random walk with constant speed of organisms (or cells). The temporal dynamics of
the automaton is defined by rotation and propagation operators together with a ‘biological’ operator which describes local interactions of organisms (or cells). The microdynamic equations are given and from these a continuous transport equation of Boltzmann type (see [2]) may be deduced. Possible applications are the swarming of the myxobacteria and ants, the contractile motion of actin-myosin fibrils, as well as the formation of aggregation patterns of Dictyostelium and the mentioned pigment cell patterns in salamander larvae. Furthermore, examples of simulations are shown.

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Study of Rayleigh-Bénard Cells with a Cellular Automaton
U. D’Ortona, D. Salin, J. Banavar(1), M. Cieplak(2), R. Rybka(3)
A.O.M.C.- U.P.M.C. case 78, Tour 13,
4, pl Jussieu, 75252 Paris Cedex 05, France

We modify a 2-dimensional Boltzmann Cellular Automaton to mimic the advection of a passive or an active contaminant. If the contaminant is temperature, the gravity effect is achieved by slightly changing the flow depending on the temperature, leading to the formation of Rayleigh-Bénard convection cells. We show that the implementation of conduction is necessary to obtain a regular pattern of cells. The same study is realized in a porous medium. The porous medium is obtain by randomly putting unaccessible sites in the lattice. In this case the instability is the Rayleigh-Darcy’s one. (1) Penn-State Univ. 104 Davey Laboratory, University Park, PA16802, USA
(2) Institute of Physics, Polish Academy of Sciences, 02-668 Warsaw, Poland
(3) Institute of Geophysics, Polish Academy of Sciences, 01-452 Warsaw, Poland
Comparisons of Lattice Boltzmann Methods with a Finite Difference Method for a 2-D Burgers Equation

Bracy H. Elton
Computational Research Division
Fujitsu America, Inc.
3055 Orchard Drive
San Jose, CA 95134-2022, USA

We look at three lattice Boltzmann methods and an analogous second-order finite difference method for solving a two-dimensional scalar, viscous Burgers equation with periodic boundary conditions. Specifically, we compare the four methods in terms of convergence attributes, including domain of monotonicity, order of convergence, and absolute errors, and in terms of their performance characteristics, including performance and timing measurements and memory requirements, on Fujitsu supercomputers.

Latice Gas Automaton Model for the Coupling between Internal and Translational Modes

Patrick Grosfils
Laboratoire de Physique Statistique
Ecole Normale Supérieure
24 Rue Lhomond
75231 Paris, Cedex 05, France

We consider a 2-D lattice gas model in order to introduce a relaxation time for the rest particles. A computation of the spectrum of density fluctuations shows dispersion for acoustic waves together with a “Mountain” mode.

Nucleation, Domain Growth and Fluctuations in a Bistable Chemical System

Daniel Gruner*, Raymond Kapral* and Anna Lawniczak**
Department of Chemistry
University of Toronto
Toronto, Ontario, Canada M5S 1A1

** Department of Mathematics and Statistics
University of Guelph
Guelph, Ontario, Canada N1G 2W1

Phase separation and nucleation processes are investigated for a bistable chemical system. The study utilizes a reactive lattice-gas cellular automaton model to provide a mesoscopic description of the dynamics. Simulations of steady-state structure, wave propagation, and critical nucleus size using this model are compared with results based on the deterministic equations of motion. The dynamic structure factor is computed for evolution
from the unstable state and the effects of correlations are examined for early and late times. The study provides insight into these processes in a fluctuating, extended medium and also provides a test of the ability of the reactive lattice-gas method to describe the fluctuations in the system.

**Comparisons between the Lattice Boltzmann Method and Traditional CFD Methods for Two-Dimensional Cavity Flow**

*Shuling Hou*

Center For Nonlinear Studies, Los Alamos National Laboratory

Despite some applications of the Lattice Boltzmann methods in hydrodynamics and other fields, quantitative studies of the method have been limited. In this work, Lattice Boltzmann BGK model (LBBGK) has been applied to the 2D driven cavity flows for Reynolds numbers up to 10,000. Detailed comparisons between the LBBGK method and traditional methods are performed and show excellent agreement. Also, the compressibility error of LBBGK methods and their convergence rates are discussed.

**Coupling of Lattice-Gas and Finite Element-Methods**

*Manfred Krafczyk*

Lehretuhl NMI, GB II

Universität Dortmund

August Schmidt Str. 8b

4600 Dortmund 50, Germany

In the last decade there has been a very successful development of Lattice Gas (LG) algorithms for simulation of flow-problems and related topics parallel to the refinement of “classical” methods like Finite Differences, Finite Elements (FE) and spectral methods. Due to their inherent structural differences LG- and FE-algorithms show specific advantages and disadvantages when imposing them on specific parts of e.g. multiphase-flow-problems governed by the incompressible Navier-Stokes-Equations. The main difference can be recognized in the fact that LG-methods are strictly local algorithms while FE-methods proceed (typically) in a non-local way. While analyzing problems where both local and non-local interactions are equally important, it is evidently desirable to couple both algorithms in order to gain the advantages of both formalisms so that the efficiency of simulations is increased. In order to demonstrate the improvement when using a “mixed” algorithm we implemented the so-called Immiscible Lattice Gas (ILG, Gunstensen & Rothman, '91) in its Galilean invariant form and coupled it with a FE-program for field computations. We show convergence-acceleration which steams directly from the physically motivated coupling of FE + ILG - Algorithms.

**Fractal Character of a Chemical Wave Front**

*A. Lemarchand, A. Lesne, A. Perera, and M. Moreau*

Laboratoire de Physique Théorique des Liquides

Université Pierre et Marie Curie

4, Place Jussieu,
A reactive lattice gas cellular automaton model is used to simulate a chemical wave front propagating in a two-dimensional (2-D) medium. The corresponding macroscopic description is given by a reaction-diffusion equation first studied by Fisher and Kolmogorov, Petrovsky, Piskunov in the 1-D case. The computed value of the front propagation velocity agrees with the 1D macroscopic value.

On the contrary, the front width is half the predicted 1-D value. This result is explained by the fractal character of the interface. The fractal structure, described through several fractal dimensions, is shown to be independent of the reaction and diffusion parameter values.

Building Correct and Stable Models for Lattice Boltzmann Hydrodynamics
Guy R. McNamara
LLNL, L-540
P.O.Box 808
Livermore, CA 94550, USA

The Lattice Boltzmann (LB) method of computational fluid dynamics has shown particular promise for modeling systems involving complex boundaries or multiphase fluids, and has proven suitable for modeling high Reynolds number flow. The original LB models suffered from defects inherited from their lattice gas ancestors, but these may be overcome by modifying the model’s equilibrium mass distribution. We describe a method of constructing LB models which makes explicit the lattice symmetries required for correct hydrodynamics. This methodology may be employed to quickly and mechanically generate collision operators, with or without energy conservation, for a variety of lattices. The LB models so constructed may not exhibit numerical stability in the limit of small transport coefficients, but in some cases this difficulty may be resolved by introducing additional lattice velocities and appealing to the principle of entropy maximization to extend the equilibrium distribution to the augmented velocity set.

Multidimensional Pattern Formation Has an Infinite Number of Constants in Motion
Mark B. Mineev-Weinstein
Center for Nonlinear Studies
Los Alamos National Laboratory
Los Alamos, NM 87545

Extending our previous work on 2D growth for the Laplace equation we study here multidimensional growth for arbitrary elliptic equations, describing inhomogeneous and
anisotropic pattern formations processes. We find that these nonlinear processes are governed by an infinite number of conservation laws. Moreover, in many cases all dynamics of the interface can be reduced to the linear time-dependence of only one “moment” $M_0$ which corresponds to the changing volume while all higher moments, $M_1$, are constant in time. These moments have a purely geometrical nature, and thus carry information about the moving shape. These conserved quantities are interpreted as coefficients of the multipole expansion of the Newtonian potential created by the mass uniformly occupying the domain enclosing the moving interface. Thus the question of how to recover the moving shape using these conserved quantities is reduced to the classical inverse potential problem of reconstructing the shape of a body from its exterior gravitational potential. Our results also suggest the possibility of controlling a moving interface by appropriate varying the location and strength of sources and sinks.

A New Class of Nonsingular Exact Solutions for Laplacian Pattern Formation

Mark B. Mineev-Weinstein
Center for Nonlinear Studies
Los Alamos National Laboratory
Los Alamos, NM 87545

We present a new class of "N-finger-like" exact solutions for the so-called Laplacian Growth Equation describing the zero-surface tension limit of a variety of 2D pattern formation problems. We prove that, contrary to the typical situation in the zero-surface tension limit, these solutions are free of finite-time singularities (i.e. they do not develop cusps in a finite time). In the long-term asymptotics the moving interface consists of $N$ separated fingers. This evolution from a quite arbitrary initial interface resembles the $N$-soliton solution of classical integrable PDE’s such as KdV, NLS, etc.

A New Technology for Fluid Simulation

Kim Molvig
Exa Corporation
125 Cambridge Park Drive
Cambridge, MA. 02140, USA

Huge increases in computing power are known to be needed for fluid flow simulation. The complexity of flow around an automobile or other object moving at a realistic speeds involves so many degrees of freedom that present methods and technologies cannot begin to provide enough computational power for accurate simulation. Exa Corporation has developed an algorithm and architectural support that together comprise a new, inherently scalable technology for fluid simulation which promises dramatic improvements in computational power - from a workstation-sized engine delivering 50x the fluids simulation performance of a Cray supercomputer initially to a PetaFlops-equivalent server ultimately. Such power is required to accurately model all the scales of motion for realistic flow speeds; five of the ten Grand Challenge problems can be directly addressed with this technology. This method represents a major advance in Lattice Gas theory - all discreteness artifacts
have been removed. The system behaves as though the underlying lattice were actually erased from the dynamics. The algorithm is fundamentally more accurate than discretized approximations to the Navier-Stokes equations, it is easier to apply as it uses a simple rectilinear grid, it is computationally much more efficient than methods based on floating point arithmetic, and it is inherently parallel.

The technology is based on a direct representation of physical fluids as a three-dimensional “board game” in which markers move and collide under a set of rules derived from this extension to Lattice Gas theory - mass, momentum, and energy are conserved exactly and for all time. Binary-encoded fluid cells, or “voxels,” take the place of floating point numbers as the fundamental unit of representation, and a small set of primitive operations on voxels takes the place of “multiply” and “add.” This new representation requires 1000 times fewer bit operations than existing floating-point based methods to compute comparable results. This fundamental efficiency can be realized through the construction of a “fluids co-processor,” the complexity of which is nearly identical to that of a floating point co-processor. Many such fluids co-processors can be interconnected to form a simple, scalable parallel system.

We present the basic principles of the technology and demonstrate its accuracy by comparing simulation results to laboratory observation for flows exhibiting separation and vortex shedding.

Transport and Diffusion in a Model Fluctuating Medium
M. Moreau, B. Gaveau, M. Frankowicz and A. Perera*
*Laboratoire de Physique Théorique des Liquides
Université P. et M. Curie, Bolte 121, 75252 PARIS (France)
*U. F. R. de Mathématiques, Université P. et M. Curie, PARIS
**Faculty of Chemistry, Jagiellonian University, KRAKOW (Poland)

Our purpose is to model the motion of a particle in a time dependent medium where the fluctuations of the medium are spatially uncorrelated but have a finite correlation time, so that it is needed to keep the past trajectories of the particle in memory in order to describe its future evolution. The medium is represented by one and two dimensional lattices. Each node of the lattice fluctuates between two internal states according to a random telegraph process. A particle moves on the lattice and obeys to a given stochastic process between the nodes. It is diffused by the nodes, the diffusion law of a node depending on its internal state. The model interpolates between a random walk with persistence and percolation problems, according to the values of the relaxation frequency and of other parameters. It can be used for the microscopic theory of reaction constants in a dense phase, or for the study of diffusion or reactivity in a complex medium.

In different cases, the transmission probability of the medium is computed exactly. It is shown that the memory effects decrease the transmission probability of the medium. Furthermore, stochastic resonances can occur, an optimal transmission being obtained for a convenient choice of parameters. In more general situations, approximate solutions are given in the case of short and moderate memory of the obstacles and shown to agree with numerical results. The diffusion in an infinite two-dimensional lattice is studied, by
computer simulations and the memory is shown to affect the distribution of the particles rather than the diffusion law.

**Long Memory Effects in the Stress Correlation Function**

Toyoaki Naitoh  
School of Business Administration, Senshu University  
Higashimita, Tama-ku, Kawasaki, 214, Japan  
and  
Matthieu H. Ernst  
Institute for Theoretical Physics, The University of Utrecht  
Princetonplein 5, P. O. Box 80006, 3508 TA, Utrecht, The Netherlands

The stress correlation function (SCF) in a one-dimensional cellular automata-fluid is calculated by computer simulations up to 3000 time steps. The results are compared with the 1-D tails $t^{-1/2}$ and $t^{-2/3}$ of bare (BMC) and self-consistent (SCMC) mode coupling theories. The crossover between both tails is estimated to occur after $t_{\text{cross}} \approx 35000$ time steps. For $t < 400$ and systems with $L \geq 500$ sites there is good agreement with BMC-theory for finite systems. For $t > 400$ there are signs of faster-than-$1/\sqrt{t}$-decay in the SCF. The simulated data for the “divergent” transport coefficient at times $t > 400$ are analyzed in terms of a crossover function, constructed from SCMC-theory. However a quantitative verification of the SCMC-theory is still out of reach.

**An Immiscible Lattice Gas in Three Dimensions**

John F. Olson and Daniel H. Rothman  
Department of Earth, Atmospheric and Planetary Sciences  
Massachusetts Institute of Technology  
Cambridge, MA 02139

We present a simple scheme for constructing collision rules for surface tension in the framework of the 4-D FCHC lattice gas. Our rule, constructed in analogy with earlier work for surface tension in lattice-Boltzmann models, acts to maximize the difference between the component of pressure normal to interfaces with the component of pressure transverse to interfaces. The model exhibits a phase separation transition at the critical reduced density, $d \approx 0.1$. We have measured surface tension and compared it with a crude theoretical approximation. We also discuss the isotropy of the surface tension.

**Pattern Formation in Phase Transition**

Yue Hong Qian and Steven A. Orszag  
PACM, Fine Hall  
Princeton University  
Princeton, NJ 08544, USA

There is an increasing interest in modeling complicated phenomena by using simple models, lattice models (lattice gas, lattice Boltzmann and lattice LBGK) are examples among others. Phase transition has been a complicated and attractive problem. Most of
the numerical simulations are based on Ising model, which is one of the simplest models in physics. The introduction of lattice gas [1] for incompressible hydrodynamics provides some possibility of studying phase transition by using a non-local interaction [2]. Phase separation models have been intensively studied by Rothman’s group at MIT [3]. By using lattice BGK models [4], we are able to demonstrate the existence of phase transition with or without surface tension. Van der Waals equation is one of the examples. We are interested particularly in the pattern formation of droplets or bubbles: the dynamical phase transition. The theoretical critical point and phase diagram are confirmed by numerical simulation. Different “pseudo-potential” which can lead to a non-monotone pressure in function of density are used to test the sensitivity of the behavior near the critical point. A universal scaling with an exponent -1/2 is obtained for the first time [5]. Numerical results also concern the surface tension and correlation function of density. We present at the same time models for one, two and three dimensions. We will discuss the applications and generalizations of our models. The treatment of wettability will be included and the multi-fluid systems without the optimization procedure will be outlined.

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Correlation of Experimental Data with Computational Data Generated by Fine-Grain, Fixed-Grid Calculations

Mr. Peter P. F. Radkowski III
Radkowski Associates
P. O. Box 1121
Los Alamos, NM 87544

Fine-grain, fixed-grid calculations have been correlated with recent (2/93) hypervelocity impact debris clouds. The non-equilibrium processes of the debris cloud formation (for example, the contemporary formation of (i) exothermic sublimation products and (ii) inert, solid fragments) greatly hinder the modeling of critical local post-perforation effects (for example, the discontinuous application of debris cloud impulses). The author uses the interactions of a large population of particles to model the initial impact, chemical reaction, and post-perforation characteristics of the observed test phenomena. Correlation with measured test data include: axial and radial velocity and momenta; and mass distribution (comparison of actual dynamic radiographs and simulated computational radiographs). Traditional Eulerian calculations are included to highlight the performance of the fine-grain model. Ongoing and near-term utilization of fine-grain calculations to model other experimental data will be summarized.
Structure of Shock in Boghosian-Levermore Automaton

K. Ravishankar
Department of Mathematics
SUNY
New Platz, N.Y 12561, USA

We classify the stationary measures of the Boghosian- Levermore automaton and study the hydrodynamics in Euler regime for the asymmetric case. We prove a law of large numbers for the location of the microscopic shock position when the initial profile is a step function. The results are obtained using the coupling methods introduced by Ferrari, Kipnis and Saada for the asymmetric simple exclusion.

Self-Organization Induced by a Differential Flow

A. Rovinsky and M. Menzinger
Department of Chemistry
University of Toronto
Toronto, Ont. M5S 1A1, Canada

A new mechanism is described that is believed to play an important role in the generation of spatiotemporal patterns in natural and artificial systems. A differential bulk flow of key species destabilizes the homogeneous steady state of certain kinetic systems with feedback and gives rise to traveling waves. The Differential Flow Induced Chemical Instability (DIFICI) is related to the Turing instability which is recognized for its central role in development and morphogenesis. DIFICI may occur in a broad class of systems, from chemical to biological and ecological.

Simulation of Fines Migration and Accumulation in Two Dimensional Porous Media Using Cellular Automata

Maurice Shevalier and Ian Hutcheon
Department of Geology and Geophysics
The University of Calgary
Calgary, Alberta
T2N 1N4, Canada

The migration and accumulation of fines in pore spaces is a major problem for the oil industry as it can lead to a decrease in the porosity and permeability of the reservoir, which ultimately causes an increase in operating costs and possibly lower rates of production. The purpose of this study is to simulate fines migration and accumulation in two dimensional porous media using a cellular automaton.

Experimental work on fines migration in two dimensional glass micro- models was carried out (Hutcheon et al. 1989, Goldenberg et al. 1989). From this work it was found that fines tend to accumulate in the pore spaces, causing a decrease in the permeability. Also, it was found that particle migration is controlled by fluid composition and velocity. Further,
when bubbles are introduced into the system, particle redistribution and transportation occurs. Finally, it was found that structures of clay particles can form across the pore throats along the gas-liquid interfaces resulting in a decrease in the permeability.

To date, there has not been a comprehensive fundamental study of fines migration in porous media. The purpose of this study is to simulate fines migration and accumulation in a two dimensional porous media using a cellular automaton.

This study will consist of the study of fines migration in a fluid. To date the study has considered fluid flow in porous media as well as the flow of "simple" fines particles, i.e. particles that do not interact electrostatically with each other. Future work will study the interaction of the fines with the walls of the porous media as well as with each other, the interaction between bubbles and fines particles and the effect solution composition has on both fines and fines-bubble migration.

Fundamental principles of fluid dynamics, fluid chemistry, colloid science and electrostatic attraction will be applied to model fines migration in a porous media. It hoped that a fundamental understanding of fines transport in two dimensions will be obtained.

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Minimally Constrained Lattice Gas Model
Doug Shim, Tim Spanos, David McEhlaney and Norman Udey
Department of Physics
University of Alberta
Edmonton
Alberta, Canada T6G 2J1.

A lattice gas model has been constructed on a 2-D lattice based solely on the premise that by removing all constraints except for conservation of energy, momentum, and mass, the macroscopic physical description will appear naturally. In this model the events which occur at lattice sites represent the probability of an event occurring in a region of space ascribed to that point and during an interval of time. The model allows for floating-point speeds, and the particles although constrained to move along the lattice acquires floating-point trajectories. At present we have demonstrated that the particle speeds evolve to a stationary 2-D “Maxwell-Boltzmann” type distribution yielding a clear definition of temperature and the concept of an internal energy. The flow described by this model is identical to the predictions of the Navier-Stokes equation. Simulation runs on this model include phase-separation of two immiscible fluids, Rayleigh-Taylor instability, flow through 2-D porous medium, and diffusion-limited aggregation growth.

Near-Criticality in a Lattice Predator-Prey Model
We study the dynamics of “Wa-Tor”, a predator-prey model on a square lattice; the parameters are the breeding rates of the predators and prey, and the predator starvation rate. The model is robust, evolving to oscillatory, phase-shifted populations of both species for a large range of parameter values, although the frequency spectrum is broad due to the randomness of the model. The most interesting result of the simulations is that the distribution function $D(s)$ of the prey cluster sizes $s$ is almost critical at large cluster sizes; it is well described by the power-law form $D(s) \propto s^\beta$, which is, however, cut off at a size $s_{co}$ (generally greater than 1000); the exponent $\beta \simeq 1.3 \pm 0.2$ is weakly dependent on the parameters of the model. The age distribution of the prey is exponential, with the lifetime essentially a function of the prey breeding rate alone.
Simulation Validations of Flows Around Circular Cylinders and the Ahmed Body
Chris Teixeira
Exa Corporation
125 Cambridge Park Drive
Cambridge, MA. 02140, USA

Simulation studies using a lattice gas algorithm (LGA) are presented for circular cylinder flows over a wide range of Reynolds numbers (Re). The LGA used has the property that it effectively erases the underlying lattice from the macrodynamics allowing the model to reproduce the results of continuum hydrodynamics exactly. For low Re flows ($Re < 100$), we demonstrate the accurate reproduction (to within the error of experimental observation) of drag coefficients and eddy-length to diameter ratios for $Re < 45$ and accurate Strouhal number reproduction for $Re > 45$ where vortex shedding occurs. The onset of vortex shedding from a steady system occurs naturally for this LGA at a $Re = 45$, the same value as found experimentally. This is in contrast to CFD results which show significant discrepancies with experimental results in this range of Re and require artificial perturbation of the flow in order to initiate shedding. Accurate reproduction of flow properties around a cylinder and an Ahmed body (crude car shape) at Reynolds numbers of practical interest, ($Re 10^6$) will also be presented.

Monte Carlo Techniques in the Lattice-Boltzmann Applications
Adnan Taymaz$^1$ and Ayse Zehra Aroguz$^2$
$^1$Physics Department, Faculty of Science Vezneciler Campus
$^2$Chemistry Department, Faculty of Engineering, Avcilar Campus
Istanbul University 34459 Istanbul, Turkey

The energy fluence parameters of interest at given points in a medium have been calculated using Monte Carlo simulation. The Boltzmann equation solution for given physical phenomenon has been obtained. The uncertainty in Boltzmann equation solution of a physical model have also been analyzed and compared in two dimension with the Boltzmann transport equation solution. In the calculation a series of sampling techniques is used and better sampling techniques has been developed.

Application of the Lattice Boltzmann Gases to Cooling Down of Cut Flowers
R. van der Sman
Agrotechnological Research Institute
Wageningen, The Netherlands

For modeling the cooling down process of packaged cut flowers by forced air convection the technique of Lattice Boltzmann Gasses is investigated. The technique seems to suit our requirements for the modeling technique. These requirements are:

- The modeled system can be built with elementary building blocks with local interaction.
- Easy refinement of the model is possible.
- The modeling technique is generable applicable to transport phenomena.
- Complicated geometries of packages are easy to model.
- The modeling technique should have an intuitive feel; i.e. should have a resemblance of the conceptual model of the scientist.

A 1-dimensional and 2-dimensional model describing the velocity field and the heat and water vapor transport will be presented. The cut flowers will be modeled as a porous medium, for which Darcy’s law is applied. Transport of heat and water vapor from the flowers will be modeled as scalars convected by the velocity field.

Commutation of Cellular Automata Rules
Burton Voorhees
Faculty of Science
Athabasca University
Box 10,000
Athabasca, AB
CANADA T0G 2R0

Let X be the global operator representing a given cellular automata rule. It is shown that the set of all cellular automata rules which commute with X is determined by the solution set of a system of non-linear Diophantine equations. Some consequences of this are discussed.

Pattern Formation in Lorentz Lattice Gas Cellular Automata
F. Wang, E. G. D. Cohen
The Rockefeller University
1230 York Avenue,
New York, NY 10021, USA

Previous investigations of Lorentz Lattice Gas Cellular Automata (LLGCA) involved the motion of a point particle along the bonds of a lattice, whose sites were randomly occupied (fully or partly) by two types of scatterers: either left or right reflecting mirrors or left or right turning rotators. New types of diffusive behavior of the particles through the scatterers were discovered[1,2,3]. In case the lattice is fully occupied by only one type of scatterers, the motion of the particle shows pattern formation, where propagation or other types of regular motion occur. A number of examples will be given.

References
1. X. P. Kong, E. G. D. Cohen, Phys. Rev. B, 40, 4838 (1989).
2. X. P. Kong, E. G. D. Cohen, J. Stat. Phys., 62, 737 (1991).
3. F. Wang, E. G. D. Cohen, “Diffusion in Lorentz Lattice Gas Cellular Automata: the hexagonal and quasi-lattices compared with he squares and triangular lattices”, (to be published).
New Class of Cellular Automata for Reaction-Diffusion Systems Applied to the CIMA Reaction

Joerg Richard Weimar
Université Libre de Bruxelles
Service du Chimie Physique, C.P. 231
Université Libre de Bruxelles
B-1050 Bruxelles, Belgium

I present a class of cellular automata (CAs) for modeling reaction-diffusion systems. The construction of the CA is general enough to be applicable to a large class of reaction-diffusion equations. The automata are based on a running average procedure to implement diffusion, and on a probabilistic table-lookup to implement the reaction. As an example application I present the Lengyl-Epstein model for the chlorite-iodide-malonic acid reaction (CIMA), which exhibits a rich set of behaviors: oscillations, hexagonal structures, stripes, oscillations, and spirals. I investigate cases showing mixed states, in which different structures coexist in space: isolated spots, isolated regions of hexagons in a surrounding homogeneous region, coexistence between stripes and oscillations, and hexagons and stripes. The cellular automaton approach has the following advantages: fast simulations of large systems, simple introduction of noise in the system, and the possibility find the connections to other, more phenomenologically constructed CAs.

A Single Lattice-Gas Cellular Automaton Model for Lasers

Xiao-Guang Wu
Department of Chemistry
University of Toronto
Toronto, Ontario, Canada M5S 1A1

A lattice-gas cellular automaton model is constructed for perfectly tuned, one-mode lasers. The model is fully discrete. A photon representation is used to describe the electromagnetic field. The atom-field interaction is treated by probabilistic updating rules that are designed on the basis of rate equation theory. This model incorporates diffusive motion (random walk with exclusion) of active particles in the dynamics so one is able to study diffusion effects on spatial hole burning.

Thermohydrodynamic Lattice-Gas Simulation on the CAM-8

Jeffrey Yepez*
Atmospheric Sciences Division, Phillips Laboratory
Hanscom AFB, MA 01731-5000, USA

Much progress has been made in recent years towards developing lattice-gas automata (LGA) and lattice Boltzmann methods for modeling hydrodynamic systems. Multiphase models have shown the ability of lattice-gases to undergo a liquid-gas phase transition where the lattice-gas simulates an attractive central force giving rise to a van der Waals type
equation of state [1]. Multispeed models have also been shown to produce thermohydro-
dynamic behavior—the report of such a multispeed lattice-gas showing a Rayleigh-Bénard
convective instability is a good example [2]. Very recently, the MIT cellular automata
machine (CAM-8) prototype has been constructed and offers an economical computational
opportunity where lattice-gas simulations can be run at high site-update rates, on large
spaces, with video-rate display graphics. These several confluent events have stimulated us
to investigate the practicality of the lattice-gas methodology for simulating certain “messy”
aspects of atmospheric dynamics. Our initiative explores lattice-gas methods related to at-
mospheric dynamics and, will involve the construction of a billion-site massively parallel
CAM. Here we present a two-dimensional test case where we have implemented on the pro-
totype CAM-8 a multispeed LGA model with gravitational forcing, temperature sources
and sinks, and free-slip and no-slip boundaries. We illustrate the flow dynamics with the
Rayleigh-Bénard convective instability. We present kinematic shear viscosity measurements
in Poiseuille flow for this thermohydrodynamic gas. We also present exponential number
density distributions under non-Boussinesq equilibrium conditions. Finally we present an
implementation of a multiphase thermohydrodynamic gas.

1. C. Appert and S. Zaleski, “Lattice Gas with a Liquid-Gas Transition”, Phys. Rev. 
Letts., 64, No. 1, 1-4 (1990)

2. S. Chen, H. Chen, G. D. Doolen, S. Gutman, and M. Lee, “A Lattice Gas Model for
Thermohydrodynamics” , J. Stat. Phys., 62, Nos. 5/6, 1121-1151 (1991)

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Simulation of Gas Flow Using a Multi-Speed LBE Model
Chen Yu
Thermal Engineering Lab
Department of Nuclear Engineering
Faculty of Engineering
Phone(Office): 03-3812-2111
The University of Tokyo
Tokyo, Japan

A class of multi-speed lattice Boltzmann models were extended into the compressible
limit. We added one degree of freedom into the sound speed of the modeled fluid, with
the use of rest particles and particle reservoir. Furthermore, the sound speed is formalized
to be dependent on thermodynamic variable(density) in the way the perfect gas does in
adiabatic case. Hence realistic gas flows under isentropic condition could be simulated
and some unphysical phenomena occurred in the simulation of compressible flow with the
previous models could be corrected.
PROGRAM

TUESDAY, JUNE 08, 1993:

MORNING SESSION  Chairperson: B. Alder

8:50–9:00  Opening Remarks: Director of The Fields Institute

9:00–10:00  M. Henon, CNRS Observatoire de Nice, France
            “Lattice Gas without Semi-Detailed Balance”

10:00–10:20  COFFEE BREAK

10:20–11:20  F. Hayot, Ohio State University, USA
            “Vortex Street in Lévy Walk”

11:20–12:20  A. Noullez, Princeton University, USA
            “Collision Rules for Two-Dimensional Hydrodynamics”

12:20–1:40  LUNCH BREAK

1:40–3:10  POSTER SESSION: THE FIELDS INSTITUTE

AFTERNOON SESSION  Chairperson: P. Lavallee

3:20–4:20  N. Margolus, Massachusetts Institute of Technology, USA
            “CAM-8: A Computer Architecture Based on Cellular Automata”

4:20–4:40  COFFEE BREAK

4:40–5:40  S. Succi, IBM Center for Scientific and Engineering Computing, Italy
            “Two and Three-Dimensional Simulations of Rayleigh-Bénard
            Turbulence with Lattice Boltzmann Method”

5:40–6:40  G.D. Doolen, Los Alamos National Laboratory, USA
            “Future Computers and Lattice Methods;
            Multiphase Flows Through Porous Media”

7:00–    DINNER AT THE WATERLOO INN

WEDNESDAY, JUNE 09, 1993:

MORNING SESSION  Chairperson: S. Succi
9:00–10:00  D. Rothman, Ecole Normale Supérieure, France
“Surface Tension and Immiscible Lattice Gases”

10:00–10:20  COFFEE BREAK

10:20–11:20  C. Appert, Université Pierre et Marie Curie, France
“Large Liquid-Gas Models on 2D and 3D Lattices”

11:20–12:20  D. d’Humières, Ecole Normale Supérieure, France
“Exact Solution for Lattice Boltzmann Equation: Boundaries and Interfaces”

12:20–1:40  LUNCH BREAK

1:40–3:10  POSTER SESSION: THEFIELDS INSTITUTE

AFTERNOON SESSION  Chairperson: A. De Masi

3:20–4:20  E.G. Flekkøy, University of Oslo, Norway
“Lattice BGK Model for Miscible Fluid Flow: Experiments and Simulations”

4:20–4:40  COFFEE BREAK

4:40–5:40  M. Ernst, University of Utrecht, Netherlands
“Metastability and Pattern Formation in Biased Lattice Gases”

5:40–6:40  R. Rechtman, Universidad Nacional Autonoma de Mexico, Mexico
“Lattice Gas Transport in Porous Media”

THURSDAY, JUNE 10, 1993:

MORNING SESSION  Chairperson: R. Desai

9:00–10:00  S.R.S. Varadhan, Courant Institute, USA
“Asymmetric Mean Zero Random Walk with Exclusion: Self Diffusion”

10:00–10:20  COFFEE BREAK
10:20–11:20  E.G.D. Cohen, Rockefeller University, USA  
“Propagation and Pattern Formation in Lorentz Lattice Gases”

11:20–12:20  A. De Masi, Università degli Studi di L’Aquila, Italy  
“Glauber Evolution with Kac Potentials”

12:20–1:40  LUNCH BREAK

1:40–11:00  TRIP TO NIAGARA FALLS

FRIDAY, JUNE 11, 1993:

MORNING SESSION  Chairperson: M. Moreau

9:00–10:00  X.-G. Wu, University of Toronto, Canada  
“Reactive Lattice-Gas Automata and Chemical Chaos”

10:00–10:20  COFFEE BREAK

10:20–11:20  S. Ponce–Dawson, Los Alamos National Laboratory, USA  
“Lattice Boltzmann Simulations of Pattern Formation Reaction-Diffusion Systems”

11:20–12:20  B. Hasslacher, Los Alamos National Laboratory, USA  
“Lattice Gases and New Emergent Complexity in Biochemical Systems”

12:20–1:40  LUNCH BREAK

AFTERNOON SESSION  Chairperson: M. Ancona

1:40–2:40  S. Chen, Los Alamos National Laboratory, USA  
“Lattice Boltzmann Method and its Application to Computational Biology”

2:40–3:40  D. Dab, Université Libre Bruxelles, Belgium  
“Polimerization through Heterogeneous Catalysis: a Reactive Lattice-Gas Automaton Approach”

3:40–4:00  COFFEE BREAK

4:00–5:00  R. Monaco, University of Genova, Italy
“The Discrete Boltzmann Equation for Gases with
Bimolecular or Dissociation-Recombination Reactions”

5:00–6:00 VIDEO SESSION

6:10–8:00 DINNER: UNIVERSITY CLUB, UNIVERSITY OF WATERLOO

8:10–10:00 ROUND TABLE DISCUSSION: THE FIELDS INSTITUTE

Moderator: B. Alder
Round Table Members: B. Boghosian, J.P. Boon, G.D. Doolen,
K. Molvig, D. Rothman

Topics: 1. Lattice gas automata and statistical mechanics.
2. Lattice Boltzmann vs. lattice-gas models:
   their applications to science and engineering.
3. Lattice gas automata and special-purpose computation.
4. Commercial applications of lattice gas automata.

SATURDAY, JUNE 12, 1993:

MORNING SESSION Chairperson: D. d’Humieres

9:00–10:00 E. Presutti, II Università degli Studi di Roma, Italy
“Critical Fluctuations in Spin Systems”

10:00–10:20 COFFEE BREAK

10:20–11:20 J.P. Boon, Université Libre Bruxelles, Belgium
“Fluctuation Correlations in Lattice Gas Automata”

11:20–12:20 B. Boghosian, Thinking Machines, USA
“Correlations and Renormalization in Lattice Gas Automata”

12:20–2:00 LUNCH: UNIVERSITY CLUB, UNIVERSITY OF WATERLOO