ABSTRACTS FOR THE JUNE 27-29, 1994 Princeton Conference
DISCRETE MODELS FOR FLUID MECHANICS

Particle Hydrodynamics
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Several particle methods such as molecular dynamics, lattice gas, lattice Boltzmann and Bird will be compared to Navier–Stokes continuum hydrodynamics as to their relative advantages and disadvantages. Particularly, the simulation of the “consistent” Boltzmann and its Enskog extension will be discussed.

Bubble Dynamics Model for Hydrodynamically Unstable Interfaces
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Evolution of the Rayleigh–Taylor unstable interface is known to be dominated by bubble growth and merging processes (1,2). Models that have been developed describe the unstable front as composed of many bubbles (the basic particles) which are rising in the gravitational field (the one–body dynamics) and merging (the two–body dynamics), where larger bubbles absorb smaller bubbles. A new statistical model has been developed(3,4). The new model is based on the Sharp–Wheeler–Glimm models(1), and incorporates the basic feature of single–bubble rise and two–bubble competition using an extended Layzer potential flow model for large density ratio(\(A = 1\)) and incompressible fluids. The model offers a unified treatment of the Rayleigh–Taylor and the Richtmyer–Meshkov instabilities. The merger model dynamics for both
instabilities are shown to reach a scale invariant regime. For the RT instability, the model predicts a constant acceleration of the front, growing as \(0.05gt^2\), while for the RM instability the model predicts a new novel scaling behavior for the bubble front, growing as \(at^{0.4}\). The model results are in good agreement with experimental and 2d hydrodynamic simulations.

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**Multiphasic Lattice Gas Models:**
**Prediction of Surface Tension and Growth Exponents**
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A liquid-gas phase separation is obtained for a lattice gas model by addition of an attractive force between particles. As the interaction does not derive from a potential, the equilibrium densities cannot be derived from the classical Maxwell’s construction. A dynamical approach allows to predict the density profile across a flat interface. The corresponding equilibrium densities and the surface tension value are in agreement with measurements on simulations [Appert, d’Humières, and Zaleski, preprint 1994].

Multiphasic lattice gas models may be applied to study spinodal decomposition. We have used the boolean model of immiscible fluids proposed by D.H. Rothman and J.M. Keller, and extended to 3D by J. Olson. Some growth exponents and power spectra scalings have been computed for several color ratios.
Hydrodynamic Limit of Lattice Boltzmann Equation
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In this talk I propose a new method to study the hydrodynamic limit of the LBE. The method employs an empirical computation of the inertial manifold for a simplified version of LBE. From the numerical results, it is possible to define the rate of convergence of LBE to the Navier Stokes equations.

Correlations and Renormalization in Lattice Gases with Chemical Reactions
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The effects of correlations in a lattice gas for the Schlögl model chemical reaction are analyzed using diagrammatic summation methods. Corrections to the equilibrium densities and diffusivities are calculated and compared to numerical experiment. The impact of the correlations on the problem of getting the lattice gas to exhibit the correct stoichiometry is elucidated.

Lattice gases with Non–local Interactions
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Lattice Gas Automaton (LGA) models with long range interactions are constructed by means of a power law distribution governing velocity configuration changes at distant nodes. Such non–local interactions mimic the effects of attractive/repulsive forces in fluid systems. The equilibrium and transport properties are considered for single– and multi–species LGA’s.
Correlations in LGA’s Violating Detailed Balance
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Non-detailed balance lattice gases exhibit strong velocity correlation in equilibrium, as measured in FCHC and FHP models. Here we present a kinetic equation, based on the BBGKY hierarchy for LGA’s, from which these equal time velocity correlations can be calculated. As a quantitative test we apply the theory to a fluid-type LGA model on a triangular lattice and to a model of interacting random walkers on a square lattice, both violating detailed balance. The numerical predictions agree very well with computer simulations.

Exact Solutions for a Semi–Continuous Model of the Boltzmann Equation
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The two–dimensional semi–continuous model of the Boltzmann equation is an integro–differential equation, obtained by assuming that all velocities have the same modulus “c”, but an arbitrary direction. For that model we built, as solitons, a family of exact solutions. Those solitons are global solutions in time of the initial value problem, and some of them correspond to partially negative initial data.

Recovery of Complete Hydrodynamics in Lattice Gas Models
Hudong Chen
Exa Corporation

We present theoretically that the correct hydrodynamics including its temperature evolution can be produced by a lattice gas model in a systematic way. The key steps are that a lattice gas system must have an independent
energy conservation law and a proper dynamic transition rate among different energy levels. By a proper choice of the transition rate and its functional dependence, it is shown that the known non-Galilean invariant artifacts in convection and pressure can be completely removed in a lattice gas model. In addition, we show that, with the removal of the above artifacts, the model automatically gives rise to the correct forms for the dissipative terms such as the viscous stress tensor and the energy dissipation. Therefore, the model produces the correct hydrodynamic equations to all relevant orders. Furthermore, it is shown, as a byproduct, the hydrodynamic temperature and the thermodynamic temperature become equivalent. The fundamental difference between this approach and the approach used for recovering hydrodynamics in the lattice Boltzmann method is that, in the former, the proper equilibrium distribution is generated by a collision process rather than being given a prescribed power series form. Hence, it will stay positive-definite in any circumstance.

An H–Theorem Without Semi–Detailed Balance
Hudong Chen
Exa Corporation

For a lattice gas system obeying Fermi-Dirac statistics but not satisfying the so-called semi-detailed balance condition, an H-theorem can still be proved if another condition for the transition matrix is used. Hence, the semi-detailed balance condition is sufficient but not necessary condition for a system to approach equilibrium. It can be seen that the new condition has a broader applicability to various lattice gas models including those which have some phase transition properties.

Growth Kinetics in Multicomponent Fluids
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The hydrodynamic effects on the late stage kinetics in spinodal decomposition of multicomponent fluids are examined using a lattice Boltzmann scheme with stochastic fluctuations in the fluid and at the interface. In two dimensions, the three- and four-component immiscible fluid mixture (with a $1024^2$
lattice) behaves like an off-critical binary fluid with an estimated domain growth of $t^{0.4\pm0.03}$ rather than $t^{1/3}$ as previously predicted, showing the significant influence of hydrodynamics. In three dimensions (with a $256^3$ lattice), we estimate the growth as $t^{0.96\pm0.05}$ for both critical and off-critical quenching, in agreement with phenomenological theory.

**Thermal Lattice Bhatnagar-Gross-Krook Model Without Nonlinear Deviations In Macro-dynamic Equations**

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We present a new thermal lattice BGK model in $D$ dimensional space for the numerical simulation of fluid dynamics. This model uses a higher order velocity expansion of Maxwellian type equilibrium distribution. In the mean time, the lattice symmetry has been upgraded to ensure isotropy for the 6th order tensor of velocity moments. These manipulations lead to macroscopic equations without the nonlinear deviations, from which conventional thermal or non-thermal lattice BGK models suffered. We demonstrate the improvements by conducting classical Chapman-Enskog analysis and by the numerical calculation of the structure of the shock wave front and the decaying rate of the kinetic energy in the shear wave flow. Parameters in the velocity expansion are given for example models in one, two and three dimensions. The transport coefficients of the modeled 1D and 2D fluids are numerically measured as well.

**New Developments in Diffusion in Lorentz Lattice Gas Cellular Automata**

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Extending the calculations of the diffusion coefficient and related quantities of a Lorentz Lattice Gas to much longer times than before, a different diffusive behavior was observed than reported before$^{[1,2]}$. One of the most striking features is that the percolation transition does not seem to have observable dynamical consequences. A survey of the present situation will be given.
Cellular Automata Modeling of Reaction–Diffusion Phenomena
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Reaction-diffusion systems have long been a subject of interest because of the complex behavior they exhibit, such as pattern formation, chemical waves, etc. The classical approach to this type of problem is to use mean-field-like partial differential equations, which are known not to describe the true behavior in low dimensions.

We present a method for simulating the microscopic dynamics of reaction-diffusion systems using probabilistic cellular-automaton algorithms. A small number of random bits at each site produce random walks, and simple synchronous update rules permit highly efficient implementation using multi-spin coding techniques and/or massively parallel machines with SIMD architecture. Moreover, these algorithms faithfully simulate the microscopic stochastic dynamics (in the limit of low density, when lattice effects become unimportant). We are therefore able to perform very precise investigations into the departure from mean-field-like behavior of such systems below their upper critical dimension.

We study the effects of the initial condition on the evolution of the system $mA+nB \rightarrow \text{[inert]}$, where $m$ and $n$ are small integers. In uniform geometry, we give examples to show that, for equal densities of $A$ and $B$ particles independently distributed, the density decays like $t^{-x}$, with $x = \min(d/4, 1/(m+n-1))$, whereas for correlated initial conditions the decay exponent is $x = \min(d/2, 1/(m+n-1))$. For a time-independent reaction front produced by opposing currents $J$ of $A$ and $B$ particles, we find that the front is described by one length scale that behaves like $J^{-\nu}$, with $\nu = \max(1/[d+1], [m+n-1]/[m+n+1])$. If space is divided into two regions, with constant initial densities of $A$ and $B$ particles respectively, a time-dependent reaction front evolves between the two regions. This front exhibits scaling behavior, with exponents related to those for the time-independent case described above, in contrast to the results reported by other authors.
Hexagonal Discrete Boltzmann Models
With And Without Rest Particles

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We compare the one hexagonal FHP\(^{(1)}\) model without rest particle, with the three hexagonal GBL\(^{(2)}\) model including rest particle and with a five hexagonal model including also a rest particle. The models with and without rest particles were called “thermal” and “athermal” models by Ernst\(^{(3)}\). For shock waves, in the parameter space building up the two equilibrium states (one parameter being the propagation speed \(\zeta\)) satisfying the Rankine-Hugoniot relations, we study whether different behaviors for the macroscopic quantities exist between the two classes. Firstly, from the knowledge of only the two equilibrium states associated to “shock profiles” solutions, we can predict\(^{(4)}\) the subdomains where the ratios \(P/M\) (\(P\) for pressure, \(M\) for mass and \(P/M\) for internal energy) are monotonic or not. Secondly, we investigate the contour maps of the mass ratio \(\rho\) across the shock and compare with the corresponding one \(\rho_C\) of the continuous theory\(^{(5)}\) (valid only for models with an infinite number of velocities as was recently emphasized by Cercignani\(^{(6)}\)). Thirdly, we seek also the subdomains where uniform solutions (densities associated to the same speed are the same at the downstream state) can exist. Our main result is that for the thermal models exist an additional subdomain including \(\zeta \simeq 0\) with curve \(\rho = \rho_C\), possible nonmonotonic \(P/M\) but without uniform solutions.

Recently for squares model\(^{(4)}\), with and without rest particles, a similar study was performed. For both squares or hexagonal models the above results are in agreement.

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Lattice Gas Models and Lattice Boltzmann Equations for Flows in Viscoelastic Media

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We shall present a family of lattice gas models displaying transverse shear waves\textsuperscript{[1]}. The corresponding lattice Boltzmann equation will be given. The common feature of all these models is the conservation of additional quantities related to the viscous stress tensor. It will be shown that a suitable coupling between this new models and the ones with only mass and momentum conservation leads to a viscoelastic behavior with transport coefficients depending on the wave vector of typical perturbations. The effects of “spurious” invariants and anisotropy will be considered.

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Trends and Opportunities in Lattice Gas Research

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Recent developments in applications of lattice Boltzmann methods to problems of industrial interest will be discussed. A probable Reynolds number upper limit of 10,000,000 for homogeneous lattice, three-dimensional hydrodynamic simulations will be outlined. Also, a summary of the usage of the lattice gas preprint library will be given. Uses of bulletin boards, research frontier summaries, and multicasting to accelerate lattice gas/lattice Boltzmann research will be presented.
We show that Lorentz lattice gases belong to the category of dynamical systems with positive Lyapunov exponents, and are therefore chaotic. As a result of the description of the Lorentz lattice gas as a dynamical system, it is possible to relate a macroscopic quantity characterizing irreversible behavior, namely the diffusion coefficient, to microscopic dynamical quantities, namely the Lyapunov exponents and the Kolmogorov-Sinai entropy, of a set of trajectories that are trapped forever in a finite region of the system. We show using arguments, based on techniques from the kinetic theory of gases, that these dynamical quantities can be explicitly computed and compared with the results of computer simulations.

Non–Gibbsian stationary states occur in dissipative non–equilibrium systems. They are closely connected with the lack of detailed balance, and the absence of a fluctuation-dissipation theorem. These states exhibit spatial and temporal correlations that are long-ranged under generic conditions, even in systems with short range interactions, provided the system has slow modes, and there is some anisotropy either in configuration space or in state space. The anisotropy may come from imposed fields (driven diffusive systems, temperature gradients). In the statistical mechanics of dissipative systems, such as stochastic cellular automata, the asymmetry is only in state space. Here the equilibrium states are non–Gibbsian, they may be spatially uniform with long range pair correlations, $g(r) r^{-d}$ (with dimensionality d), and may even exhibit instabilities, and lead to the formation of clusters or patterns.
Visualization of Dynamic Fluid Simulations: Waves, Splashing, Vorticity, Buoyancy

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We develop a visualization technique for the modeling and animation of viscous incompressible fluids. We use the full time-dependent Navier-Stokes equations to comprehensively simulate 2D and 3D incompressible fluid phenomena. Unlike previous fluid animation graphics techniques which were based on approximating solutions to fluid motion, we use these equations to accurately model shallow or deep fluid flow, transient dynamic flow, vorticity and splashing in simulated physical environments. In our simulations we can also include variously shaped and spaced static or moving obstacles that are fully submerged or penetrate the fluid surface. We model interactions of moving obstacles with other moving or static obstacles using our dynamic framework for modeling elastic and rigid objects.

We use standard stable numerical analysis techniques based on finite differences for the solution of the Navier-Stokes equations. We solve these equations by iterating an initial set of pressures and velocities defined over the finite-difference grid. To model free-surface fluids, we use a technique which is based on the Marker-and-Cell method. Based on the fluid’s pressure and velocities obtained from the solution of the Navier-Stokes equations this technique allows modeling of the fluid’s free surface either by solving a surface equation or by tracking the motion of marker particles. The later technique is suitable for visualization of splashing and vorticity, since we render the marker particles as spheres based on Silicon graphics hardware routines.

Furthermore, we develop an editing tool for easy definition of a physical-world which includes obstacles, boundaries and fluid properties such as viscosity, initial velocity and pressure. Using our editor we can perform complex fluid simulations without prior knowledge of the underlying fluid dynamic equations. Finally, depending on the application, we render the fluid’s surface and the other obstacles using well-developed graphics techniques to model transparency, texture mapping, illumination, reflectivity and object material properties. All of those techniques are implemented using standard Silicon graphics hardware routines.

We present a series of complex two- and three-dimensional simulations involving fluid animations. The first two involve splashing phenomena caused by fluids splashing into fluids, while the following three involve animations with waves and interactions of fluids with obstacles including buoyancy.
Boundary Conditions in Discrete Kinetic Theory and Applications
Renée Gatignol

The method of discretization of the velocities allows to replace the usual Boltzmann equation by a system of partial differential equations which is more tractable. By using simple models without spurious invariants, we specify the boundary conditions in two cases: first on an impermeable wall, and second on an interface with the condensation and evaporation phenomena. As applications, we consider Couette flows between two parallel infinite plates, and the evaporation and condensation problems between interfaces. With some particular models, we observe the phenomenon of temperature inversion: the temperature is strictly increasing from the hot interface to the cold interface.

First Steps towards a Description of Tracer Dispersion in Porous Media by Means of Lattice Gases
D. Grubert

The transport of particles in porous media leads to dispersion, due to the tortuosity of the path. If the scale of the heterogeneity is much less than that of the experiment, it is possible to define an REV (Representative Elementary Volume) with a constant dispersivity. In this case, Fick’s law is valid and the usual advection–diffusion equation can be applied.

In strongly heterogeneous media, it is impossible to define a REV and the dispersion becomes scale-dependent. Therefore, as a different approach, flow and transport in a porous medium are modeled on a microscopic scale by means of lattice gases.

First results of numerical experiments are presented, that simulate flow and dispersion for Hagen–Poiseuille flow and in a simple porous medium.
Internal Noise, Oscillations, Chaos and Chemical Waves
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The effects of internal noise on chemical oscillations, chaos and pattern formation processes will be described. The problem is investigated using a reactive lattice-gas automaton model for the Willamowski-Rössler reaction, a mass-action model that exhibits a period doubling cascade leading to a strange attractor. The nature of the stochastic dynamics is considered in both the period-doubling regime, where the scaling structure is analyzed, and in the regime where deterministic chaos is observed. Pattern formation and wave propagation near deterministic chaos are investigated in the fluctuating medium. The interplay among spatial degrees of freedom, system size and internal fluctuations are studied for this chaotic dynamical system.

Cellular Automaton Model Of Coupled Mass Transport And Chemical Reactions T. Karapiperis
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Mass transport, coupled with chemical reactions, is modeled as a cellular automaton in which solute molecules perform a random walk on a regular lattice and react according to a local probabilistic rule \[1\]. Stationary solid particles dissolve with a certain probability and, provided solid is already present and/or the solution is saturated, solute particles have a probability to precipitate. No a priori restriction is placed on the number of particles per lattice site. Assuming molecular chaos and a smooth spatial dependence of particle density, we obtain, in the continuum limit, the macroscopic reaction-transport equations with standard advection and diffusion terms. The model is first applied to homogeneous systems subject to the reactions \[a + b \iff c\] and \[a + b \to c\], respectively. In the reversible case we find that correlations between the reacting particles can influence the macroscopic properties of the equilibrium state (cf. \[2\]). For the irreversible reaction, the long-time decline of reactant density is slowed down because of density fluctuations that lead to segregation of the reactants \[3\]. The rate of annihilation depends on whether there is relative advection between the reactants. In the simulation of an initially separated \[a + b \to c\] system the width of the reaction zone grows faster than predicted by the reaction-diffusion equations \[4\]. The difference diminishes with enhanced diffusion, thus suggesting a density fluctuation effect similar to the homogeneous case. We also simulate autocatalytic reaction schemes \[5\] displaying spontaneous formation of spatial concentration patterns \[6\]. Our simulation of the dissolution of a solid block in a streaming fluid yields solid precipitation downstream from the original solid edge, as a result of fluctuations in solute density.
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Simulation of Properties of Elastic Solids with Lattice Gases

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Although the equations for the deformation of a linear elastic solid are well known, determination of the deformation and stress is difficult except for very simple situations. The case where the elastic solid is seeded with numerous microscopic defaults is particularly difficult to deal with, even in two dimensions, both in the laboratory and in numerical simulations. Experiments are very tedious since sample preparation and interpretation of the results are time consuming, and tests are usually destructive. Some simulations currently use analogies with electrical resistance or springs networks.

Lattice gases provide an alternative method of simulation. The basis of the method is the equivalence principle, i.e.: the equations for the displacement in a linear elastic solid are similar to the equations for the velocity in an incompressible, Newtonian fluid undergoing creeping motion. The patterns originating in a steady state fluid flow with appropriate boundary conditions can thus be interpreted to represent patterns in an elastic solid and the macroscopic properties of solids can be measured. The features of lattice gases can be exploited in this context because lattice gases permit to simulate a large number of defaults. A default is conveniently simulated in a
lattice gas as a region of very low viscosity compared to that of the surrounding fluid: a site identifying a default merely uses a different collision table than the surrounding fluid. Solids containing up to 1000 (secant and non secant) defaults were simulated with simple shear conditions; the injection of particles was arranged so that the total change of momentum required to maintain a given velocity (displacement) gradient could be measured. The graph of macroscopic properties of the solid (equivalent of Young modulus) as a function of the number of defaults was obtained and compared with published results.

**Fluctuations and Chemical Waves in Bistable Reacting System**

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A multi–species reactive lattice–gas automaton model is used to study the steady–state bifurcation structures, wave propagation in a bistable chemical system, the Schlögl model. In contrast to earlier investigations of this system, the dynamics of all three species that take part in the reaction are followed. Far–from–equilibrium constraints are imposed by feeds of two species from the boundaries, mimicking the situation that occurs in continuously–fed–unstirred reactors. As a result, a detailed examination of the effects of fluctuations and feed rate variations on the steady–state structure and pattern formation processes can be carried out.

**Shock Profiles in Lattice Models: Some Exact and Some Simulation Results**

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The full microscopic structure of macroscopic shocks is obtained exactly in the uniform one-dimensional totally asymmetric simple exclusion process. I shall also describe studies, via computer simulations, of the motion of shock fronts in a variety of other one- and two-dimensional stochastic lattice models with parallel and serial dynamics, infinite and finite temperatures and ferromagnetic and antiferromagnetic particle interactions.

The nonequilibrium stationary states of the asymmetric simple exclusion process with one site partially blocked were investigated both analytically and via simulations.
ALGE: A Supercomputer for 3-D Lattice-Gas Automata

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This paper presents the architecture of a scalable SIMD supercomputer, called ALGE, designed for high Reynolds number 3-D lattice gas simulations. ALGE consists of an array of custom VLSI processors interconnected as a 2-D torus. Each processor has direct access only to its local memory. The effectiveness of ALGE is based on a set of synergistic architectural mechanisms. The most important one is the collision unit. By exploiting the group symmetry properties inherent in the FCHC models, it reduces the size of the required collision lookup table by more than 100 times without degrading Reynolds coefficients. Other supporting architectural mechanisms include a novel address generator containing a register file and multi-dimensional modulo adders for efficient implementation of the virtual move update algorithm, extensive random number generators for probabilistic boundary conditions, transpose buffers for supporting a bit-serial word-parallel organization and address sequences optimized for efficient DRAM page-mode access, a simple and fast router for local communication, support for statistics collection, and a scalable I/O mechanism. The speedup achieved by a large scale ALGE system is very close to linear. A 2K-processor ALGE machine can be several hundred times faster than current implementations on other supercomputers such as a 64K-processor Connection Machine CM-2 or a 4-processor CRAY-2. The future evolution possibilities of ALGE will also be discussed.
Thermal turbulence in He gas at low temperature (5K) allows a broad study of different states of turbulence. By varying the gas density, the Rayleigh number can be swept from $10^3$ to $10^{15}$ and the Reynolds number can go beyond $10^7$. All the measured quantities, in each turbulent state, scale with $R_a$ or $R_e$. We will describe in detail the characteristics of soft turbulence ($R_a < 10^8$), hard turbulence ($R_a > 10^8$), and present scaling models for various models for various length scales and time scales in the problem. Room temperature study in $SF_6$ gas allows a detailed analysis of the thermal and velocity boundary layers. From such studies we will propose models for the possible asymptotic state of thermal turbulence.

**Some Recent Developments in CFD Based on Unstructured Grids**

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The numerical solution of the (continuum) equations describing flows, i.e. the Navier–Stokes equations, using unstructured, irregular grids of triangles and tetrahedra, has seen a number of recent developments. In particular, we will describe recent progress in the following areas:

- Generation of Navier–Stokes grids suitable for high-Re flows;
- Grid generation from discrete data;
- Edge–based flow solvers;
- Particle–Flow models and algorithms;
- Moving Grids;
- Parallelization;
- Link to CSD or CTD codes.

The talk will try to focus on the algorithmic aspects of each of these areas, in the hope that a stimulating discussion with the lattice gas CFD community can be established.
Physical Modeling on CAM–8
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Conventional computers are grotesquely inefficient at running CA models, and so discourage the development of these intrinsically efficient kinds of computations. To meet our own simulation needs, and to encourage others to investigate CA models, we have developed general-purpose CA machines which are optimized for studying large-scale CA systems. These machines are a small step towards harnessing the kind of computational density and speed available in nature only in a spatially local format. Given a computing medium with a physics–like structure, it is only natural to use it first to model physics itself. In this talk, I will demonstrate some of the physical modeling tasks that CA’s have been applied to on our new CAM–8 machines. I will also discuss some of the practical and theoretical modeling challenges that we are addressing with the aid of our CA hardware.

Comparison of Spectral Method and Lattice Boltzmann Simulations of Two-Dimensional Turbulence
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Methods based on the Lattice Boltzmann Equation (LBE) approach are an interesting and potentially useful alternative to traditional computational methods for simulation of fluid turbulence. The LBE method benefits from a considerable reduction in noise relative to the Cellular Automaton (CA) fluid schemes upon which they are based. In addition, recent advances in LBE methods alleviate or completely solve certain other problems that simple CA methods experience, while maintaining desirable features such as ease of implementation on vector and parallel architectures. In particular, LBE methods with pressure corrections and a single time relaxation approximation for collisions adhere to Galilean invariance, admit a well behaved equation of state, and rapidly approach local thermodynamic equilibrium in an easily controllable fashion. Using these recent advances, LBE fluid simulations schemes can be meaningfully compared with spectral method solutions to the equations of two dimensional incompressible hydrodynamics and magnetohydrodynamics (MHD). Comparisons of the methods for hydrodynamics show good (or, even excellent) quantitative agreement with regard to the evolution of bulk quantities such as energy and enstrophy, and also with regard
to energy spectra. Detailed comparison of vorticity contours and streamlines indicate that very similar structures appear in the two simulation types. The main source of the computed absolute error (relative to the spectral simulation) appears to be a spatial drift of these similar structures. Examples of MHD LBE computation using a recently developed “13 bit” representation are also presented.

**Thermal Lattice–Boltzmann Simulation of Convective Flows**

Guy McNamara  
*Center for Non–Linear Studies*  
*Los Alamos National Laboratory*  
*Los Alamos, NM*

Alex Garcia  
*Department of Physics*  
*San Jose State University*  
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We have developed a three–dimensional, 21–velocity, 4–speed, thermal lattice–Boltzmann model and have tested it on a number of simple two–dimensional flows, including Rayleigh–Bénard and slot convection. This model employs a cubic lattice with particles moving at speeds 0, 1, $\sqrt{3}$, and 2 lattice spacings per time step. Isothermal boundary conditions are implemented using an extension of the so–called reflection–principle boundary conditions for the Navier–Stokes equations. Measurements of speed and attenuation rate of traveling sound waves show excellent agreement with theory. Simulations of Rayleigh–Bénard and slot convection (with temperature ratios between the hot and cold sides of the system as high as 2:1) are compared against results from conventional finite–difference codes and show good agreement.

**Catalytic Interface Erosion**

Hsin-Fei Meng  
and  
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We study new interface erosion processes: the catalytic erosion. We consider two cases: the erosion of a completely occupied lattice by one single particle starting from somewhere inside the lattice, as well as the kinetic roughening of an initially flat surface, where ballistic or diffusion-limited particles erode the surface but remain intact themselves. Many features resembling realistic
interfaces, for example, islands and inlets are generated. The eroded regions
can have continuously tunable fractal dimension; in addition, a rich variety
of the dependence of the surface width on the system size is observed.

Digital Physics:
A New Technology for Fluid Simulation

Kim Molvig

Exa Corporation

Exa Corporation is developing a commercial package for fluid dynamics ap-
lications based on its Digital Physics Technology – an extension of the Lat-
tice Gas concept familiar to those in attendance at this conference. The
development leverages the 1000x inherent computational advantage of Dig-
tal Physics over the floating point approximations to Navier-Stokes. Digital
Physics goes beyond previously known lattice gas theory in several significant
ways that are necessary to the practical application of the method: 1) All
discreteness artifacts are removed such that the system behaves with very
high statistical accuracy like a true continuum fluid, including thermal and
trans-sonic behavior; 2) Collision efficiency has been improved to the point
that the mean free path can be reduced to a small fraction of the lattice spac-
ing, corresponding to $R^* \sim 40$; 3) Allowance is made for a variable resolution
grid – also free of discretization artifacts; 4) Noise has been reduced substan-
tially over traditional lattice gas methods making it easy to make practical
measurements of transient quantities; 5) A Shot Noise Theorem is built into
the dynamics to insure that whatever fluctuations remain have no effect on
the mean dynamics; 6) A Slip Boundary Layer technology has been de-
veloped to give low resolution access to very high Reynolds number flow regimes
including separation. These are the theoretical features of the technology. In
addition Exa is developing the hardware and software support that its vision
of a Fluid CAD (FCAD) product requires. Exa has designed and built a
custom ASIC chip and board that plugs into a Silicon Graphics workstation
to provide the capability 5,000,000 cell simulations at a performance level of
10 Cray YMP pipes. Future parallel implementations will increase performance by factors of a hundred and more. An integrated software environment
based on Parametric Technology Corporation’s Pro/Engineer, allows the user
to import or create a complex solid shape in CAD, have it compile down to
the lattice and decompose automatically for parallel execution, and visualize
the data in an SGI Explorer environment. The talk will focus on theoretical
developments, simulation results and computer architectural advantages,
and give a brief overview of Exa’s FCAD concept.
Steady Supersonic Flow in a Discrete–Velocity Gas
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Unsteady shocks are easily generated in any discrete–velocity gas (DVG) model and can be understood as serving to put the different parts of the fluid in communication. However, the limited span of the particle velocities in many DVG models precludes steady supersonic flow. A DVG model with 25 velocities in 2D and a simple extension of it to 3D is considered. The model has detailed balance and a study of the characteristics of the model–Euler equations shows that the model supports steady supersonic flow. A preliminary study of stationary shocks in the model is carried out using a robust finite–volume flux–splitting scheme for the discrete–velocity gases.

The Global Solvability for Discrete Models

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A simple and effective approach for obtain the a priori estimates for discrete kinetic models is suggested\textsuperscript{1}. This approach is based on one simple lemma which allows us to get positiveness of solution for the Boltzmann equation and its discrete models. For some class of discrete models in case of any dimensions and positive initial data the boundedness of solution and accordingly the global existence theorem are received.

\textsuperscript{1}N.Nurlybaev, Discrete velocity method in the theory of kinetic equations, TTSP 22(1), 109-119(1993).
Among the many numerical methods in fluid mechanics, cellular automata and Boltzmann lattice gases have the rather unique property of incorporating some information related to molecular dynamics. Quite early in the development of the subject this has been used to model combustion instabilities and two-phase flows, both notoriously difficult to simulate with conventional numerical methods. Other areas as well deserve to be investigated from this point of view too. I shall consider as an example of this situation the trans-sonic flows: as the previous examples, the usual numerical methods meet problems there because the equations are hyperbolic somewhere and elliptic somewhere else, making an uniform “classical” integration scheme very difficult to find (or very unstable...).
Spurious invariants exist in lattice gas and lattice Boltzmann models. They may have important influence on the dynamics of the model through the pressure term. A severe case is the study of shock wave. We shall indicate possible ways of eliminating staggered invariants for lattice BGK models. As applications, we will show a simulation of shock wave and present flow behaviors of high Reynolds numbers with or without the elimination of staggered invariants.

Lattice Boltzmann Model for Non–ideal Gases and their Mixtures

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We will present in detail the previously proposed lattice Boltzmann model for non–ideal gases and multiple components. In this model, interparticle forces are incorporated and the momentum is conserved globally. A non–ideal–gas equation of state can be derived in terms of the interparticle interaction, and when properly chosen, a liquid–gas type phase transition can be simulated. The coexistence curve, the density profile across the liquid–gas interface and surface tension are all obtained analytically and are shown to be isotropic. The diffusivity in a mixture of non–ideal gases is also obtained through a Chapman–Enskog calculation.
Lattice Boltzmann Computing: the Old Story and the New Perspectives
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The basic ideas behind the Lattice Boltzmann equation are presented together with an assessment of its potential future developments.

Numerical Simulations for Granular Flows Using Lattice BGK Models
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Many continuum theories for granular flow produce an equation of motion for the fluctuating kinetic energy density (‘granular temperature’) that accounts for the energy lost in inelastic collisions. Apart from the presence of an extra dissipative term, this equation is very similar in form to the usual temperature equation in hydrodynamics. It is shown how a lattice-kinetic model based on the Bhatnagar-Gross-Krook (BGK) approximation of the Boltzmann equation that was previously derived for a miscible two-component fluid may be extended to model the granular temperature equation. The extension is made by noting that in a two-species mixture, the equation of motion for the concentration field for one species can be made to be analogous to that for the granular temperature when a source and a sink of concentration are added. The source and sink depend only on the local properties of the fluid and correspond to the viscous heating and inelastic dissipation terms respectively in the granular temperature equation. A simulation of the extended model for the case of an unforced granular fluid reproduces the phenomenon of ‘clustering instability’, viz. the spontaneous creation of dense regions of low kinetic energy interspersed in a dilute ambient of high energy, which occurs generically in all granular flows. The success of the continuum theory in capturing this basic phenomenon, which lends credence to a proposed physical mechanism for clustering in granular flows, is discussed.
Simulation Validations of Digital Physics

Chris Teixeira
Exa Corporation

A summary of the theoretical attributes of Exa’s Digital Physics simulation engine is presented that allows it to exactly emulate both the conservation and dissipative macroscopic behavior of single phase Newtonian fluid mechanics. Simulation results for a series of benchmark fluid mechanics problems that demonstrate the quantitative validity of the model are presented including accurate reproduction of Coefficients of drag and Strouhal number for flow around circular cylinders for Reynolds number ranging from 10 to 1 million (including the drag crisis), accurate reproduction of coefficient of lift for a NACA airfoil for a range of increasing flow angles culminating with accurate capture of stall angle, and accurate reproduction of eddy-lengths beyond a backwards-facing step for a range of Reynolds numbers. Simulation results will also be presented for a series of flows around geometries of practical interest and complexity including a realistic car body provided by Ford Motor Co. and a three-dimensional internal duct system provided by General Motors.

An Engineering Fluid CAD Environment Based on Digital Physics

Kenneth R. Traub
Exa Corporation

In this poster talk, we describe and demonstrate a complete, working software environment for solving real-world fluid flow problems, based on Exa’s Digital Physics technology. Digital Physics is an extension of lattice gas technology, with these attributes of importance in solving complex flow problems: removal of all discreteness artifacts, a variable resolution grid technique, a greatly reduced level of statistical noise, and a boundary layer simulation technique which gives low resolution access to very high Reynolds number flows. The unique attributes of Digital Physics are presented elsewhere in this conference.

The main components of Exa’s Fluid CAD software system are: (1) A front-end for case construction built atop the Pro/ENGINEER mechanical CAD system from Parametric Technology Corporation; (2) An automated discretizer which converts the description of a simulation case as a solid model into lattice form; (3) A high performance simulation engine which couples the
Digital Physics simulation algorithm with Exa’s fluids accelerator hardware; and (4) A sophisticated fluid visualization environment built atop Explorer from Silicon Graphics, Inc.

We will demonstrate how a user can import a complex geometry into the CAD front end, annotate it with flow properties including simple specifications of variable resolution, submit the case for automatic discretization and simulation, and explore the results in the visualization system. We will show real-world cases obtained from Exa’s customers in the automotive industry.

Lattice Boltzmann Simulations of Laminar and Turbulent Flow Past a Cylindrical Obstacle

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We present lattice Boltzmann simulations of flow past a cylindrical obstacle. We are interested in the effect of turbulence in the incident flow on the coherence of the von Karman street.

Our study is based a Lévy walk model of turbulence in a lattice Boltzmann model. We discuss pressure around the cylinder in the laminar and turbulent regimes, as well as the dependence of the von Karman street on the analogue of integral scale in our model.

Diffusion in Honeycomb and Quasi-Lorentz Lattice Gas
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The diffusive behavior of a particle on a honeycomb and a quasi-lattice occupied randomly by fixed or flipping scatterers is discussed. A comparison with the behavior on the square and the triangular lattices will be made\textsuperscript{[1,2]}

1. E. G. D. Cohen, Fei Wang, The Fields Institute Series, Am. Math. Soc. (1994).
2. E. G. D. Cohen, in: Microscopic Simulations of Complex Hydrodynamic Phenomena, NATO Series, 92, M. Mareschal and B. L. Holian, eds., Plenum Press, New York, 137-152 (1992).

Hydrodynamical Simulations from BGK Model
Kun Xu, Luigi Martinelli and Antony Jameson
Department of Mechanical and Aerospace Engineering
Princeton University

Starting from the gas-kinetic Bhatnagar–Gross–Krook model (BGK), a new gas–kinetic scheme for the hydrodynamical compressible Euler and Navier–Stokes equations was developed.

This scheme differs from any other “Boltzmann–type schemes,” in which the integral solution of the BGK model and the collisional conservation constraints are used at the same time. Also, the continuous particle distribution function is adopted in the calculation of time–dependent numerical fluxes. In this paper, we give the basic idea of constructing this scheme and analyze its properties in terms of central–difference and upwind schemes. The similarities and differences with the Lattice Boltzmann methods are mentioned. At the end, some test cases for the 1–D and 2–D steady and unsteady gas flows are presented.

Intermittency of Dissipation Rate in Turbulence
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Incompressible Limit of Discrete Velocity Model
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Consider the discrete velocity model with random collisions on \( \mathbb{Z}^d \). The configurations at each site \( x \in \mathbb{Z}^d \) consist of particles with unit velocity in each direction. There is a hard core interaction among particles with the same velocity so that at each site there is at most one particle with a given velocity. For example, in \( d = 3 \) there are six types of particles corresponding to the six unit vectors in \( \mathbb{Z}^3 \). The dynamics consists of two parts: the asymmetric simple exclusion part and the collision part. For particle at \( x \in \mathbb{Z}^d \) with velocity \( e \), it jumps to position \( x + e' \) with rate \( \alpha_e(e') \) provided the jump does not lead to a violation with the hard core interactions among particles with the same velocity. In other words, particle at \( x \) with velocity \( e \) will jump to
$x + e'$ only if there is no particle at $x + e'$ with velocity $e$. The velocities of the particles are preserved under this dynamics so that particles with velocity $e$ remain particles with velocity $e$ after the jump. If $\alpha_e(e') = \delta(e, e')$, particles with velocity $e$ jump with rate 1 in the direction $e$ and the identification of these particles as having velocity $e$ is appropriate. Otherwise it should be considered as having velocity $\alpha_e(e')$. This is the asymmetric simple exclusion part of the dynamics.

The collision part can be described as follows. If particles with velocities $e$ and $-e$ occur simultaneously at any site $x \in \mathbb{Z}^d$, the velocities of particles change to $e'$ and $-e'$ with rate one for any direction $e' \neq e$, again subject to no violation with the hard core interaction. This is the collision part of the dynamics.

We consider the incompressible limit of this model in dimension $d \geq 3$, namely, the average density and velocity of particles are of order $\epsilon$ while the time scale of the dynamics is of order $\epsilon^{-2}$. We prove that the empirical velocity (i.e., the macroscopic velocity of the particle systems) satisfies a Navier-Stokes equation. The viscosity of the resulting equation is characterized by a Green-Kubo formula, which is then reformulated as a variational principle.