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The accomplishments of this grant include:

- i. A direct simulation Monte Carlo method for rarefied gasdynamics, patterned after the DSMC of G. A. Bird, in which molecular velocities are discretized to be integers (IDSMC) was developed. The method has been implemented on coarse-grained multi-computers such as the Intel iPSC, Symult 2010 and Intel Gamma with a self-adaptive rectangular mesh to optimize load balancing.
- ii. A finite-difference method for solving the discrete-velocity (lattice gas) Boltzmann equations has been formulated and implemented. Calculations were made of problems in heat transfer, shock wave structure and vapor deposition.
- iii. The applicability of multi-speed discrete-velocity gases to compressible flows has been examined from a fundamental point of view. The equation of state, the anisotropies and the advection velocities for multi-speed models on the square and triangular lattices were derived. It was shown that the pathologies shown by multi-speed lattice gases can be made rather small.

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- iv. A computational method has been developed in which adjacent cells in a cell network interact through an exchange of particles, commensurate with the equilibrium fluxes of mass, momentum, and energy. This corresponds to the infinite collision rate limit of the model gas, resulting in very low viscosity. The scheme is more efficient than any direct simulation with cellular automata or other method for solving the lattice Boltzmann equations.
- v. A simple multi-speed model, the nine-velocity model has been studied extensively. Solving the (inviscid) Riemann problem with the model yields almost all of the phenomenology associated with a perfect gas. An exact (viscous) shock profile is computed for the model and is compared to a Navier-Stokes shock profile. Adiabatic channel flow is simulated with the model and the results compared to an integral solution of the Navier-Stokes equation. The comparisons in both cases are excellent. It is also shown that the nine-velocity gas does not permit steady supersonic flow.

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Investigations of the Motion of Discrete-Velocity Gases

1 June, 1989 - 30 November, 1991

Principal Investigator: B. Sturtevant

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Investigations of the Motion of Discrete-Velocity Gases

1. Statement of Work

1. Develop the IDSMC for engineering use, including:
 - i. Introduce a more realistic molecular model.
 - ii. Implement diffuse-wall boundary conditions.
2. Investigate other methodologies for simplifying the treatment of molecular collisions in the IDSMC.
3. Bench mark the IDSMC with a large-scale computation of engineering importance, for example, perfect-gas flow over a sphere or cylinder.
4. Continue investigations of relaxation to equilibrium and anisotropy in the 2-D 9-velocity cellular automaton. Consider the applicability of dynamical systems theory to questions of reversibility and stability.
5. Extend the 2-D 9-velocity CA to:
 - i. 3-D 15-velocity model.
 - ii. 2-D 25-velocity model.
 - iii. 3-D 45-velocity model.
6. Extend the 2-D CA to three dimensions.
7. Compute test cases with the above models for comparison with the IDSMC and DSMC.

2. Status of the Research Effort

The accomplishments of this grant are described in the publications listed in Sec. 6 and, more recently, in the Caltech Ph.D. Thesis "A Study of Multi-Speed Discrete Velocity Gases" by Balu Nadiga. They include:

1. Development of a direct simulation Monte Carlo method for rarefied gasdynamics, patterned after the DSMC of G. A. Bird, in which molecular velocities are discretized to be integers (IDSMC). The method has been implemented on coarse-grained multi-computers such as the Intel iPSC, Symult 2010 and Intel Gamma with a self-adaptive rectangular mesh to optimize load balancing. Many problems in gasdynamics were solved as test beds and to measure performance.
2. Formulation and implementation of a finite-difference method for solving the discrete-velocity (lattice gas) Boltzmann equations. Calculations were made of problems in heat transfer, shock wave structure and vapor deposition, typically with 9- or 13-velocity models, but in one case with a 40-velocity model. As with all of our numerical direct simulations of discrete-velocity gases, most of the repetitive calculations are done only once, and the results are stored in look up tables.
3. Study of the applicability of multi-speed discrete-velocity gases to compressible flows from a fundamental point of view. The equation of state, the anisotropies and the advection velocities for multi-speed models on the square and triangular lattices are derived. Dependence on the model of any of these to leading order in the flow velocity is shown to be only through a fourth moment of the stationary equilibrium speed distribution. Thus the pathologies shown by multi-speed lattice gases can be made rather small.

4. Development of a computational scheme (EFM) in which adjacent cells in a cell network interact through an exchange of particles, commensurate with the equilibrium fluxes of mass, momentum, and energy. This corresponds to the infinite collision rate limit of the model gas, resulting in very low viscosities. The scheme is more efficient than any direct simulation with cellular automata and other methods for solving the lattice Boltzmann equations.
5. Exhaustive study of a simple multi-speed model, the nine-velocity model. Solving the shock tube problem with the model yields almost all phenomenology associated with a perfect gas. An exact shock profile is computed for the model and is compared to a Navier-Stokes shock profile. Adiabatic channel flow is simulated with the model and the results compared to an integral solution of the Navier-Stokes equation. The comparisons in both the cases are excellent. It is also shown that the nine-velocity gas does not permit steady supersonic flow.

In the following sections we describe results which have not yet been published.

3. A Method for Near-Equilibrium Discrete-Velocity Gas Flows

We have developed a simulation scheme for discrete-velocity gases based on *local thermodynamic equilibrium*. Exploitation of the kinetic nature of discrete-velocity gases results in a natural splitting of fluxes, and the resultant scheme strongly resembles the original processes. Calculation of exact molecular interactions by direct simulation is computationally intensive, perhaps unnecessarily so, and limits the maximum achievable Reynold's number. It is felt that a better simulation technique for discrete-velocity gases can be achieved by using in conjunction with the underlying concept of particles, an Eulerian picture of the flow field. The resulting scenario is one in which *cells* in a flow field, constituted by a discrete-velocity gas, interact in terms of mass, momentum, and energy fluxes at the boundaries, the currency of the interaction being the particles with the discrete-velocities. Further, if the interactions between the cells are based on the *local equilibrium* fluxes, then we have a method which is kinetic based and at the same time models the *infinite collision rate* (near-equilibrium) limit of the kinetic process. These ideas come from the equilibrium flux method (EFM) of Pullin, which is a kinetic-theory-based finite volume method for calculating the flow of a compressible ideal gas. In the EFM, the particle ensemble simulation of an ideal gas is replaced by a scheme in which adjacent cells in a cell network interact directly through exchange of mass, momentum, and energy, the exchange in t being calculated using the equilibrium flux relations.

The kinetic nature of the scheme and the modeling of the *infinite collision rate* limit result in a low value of (numerical) viscosity, whose macroscopic behavior is qualitatively like that of a viscosity resulting from molecular interactions. A first order method and two second order methods using the total variation diminishing principle are developed. An example application is presented. While this technique retains the attractive features of lattice gases — simplicity and parallel evolution, it represents a large improvement over the currently used lattice gas automata simulations and lattice Boltzmann equation solution techniques, in that the evolution is based on the inviscid, non-heat conducting limit. With this approach much higher Reynolds numbers are achievable than with any present methods, given the same computer resources. The ideas being general, the scheme is applicable to any discrete-velocity model, and to lattice gases as well.

4. An Exact Shock Solution for a Nine-Velocity Gas

The shock-structure problem, because of the absence of solid boundaries and the simplicity of the geometry, is particularly useful in studying the physics of computational models of fluids. The success of

discrete-velocity models of fluids, inclusive of a class of lattice gases, in reproducing various fluid phenomena is now well known. Most work in this area, however, has been confined to *single-speed* models, where the absence of an independent energy variable leaves the thermodynamics incomplete. While the exact structure of shock waves in such *single-speed* models are known, their counterparts in the *multiple-speed* models are likely to be more important because of the non-trivial thermodynamics.

An exact shock solution is computed in a *multiple-speed* discrete-velocity gas, the nine-velocity gas, the simplest *multiple-speed* model on the square lattice in two dimensions. The multiplicity of speeds ensures nontrivial thermodynamics. The model Boltzmann equations are solved numerically for steady one-dimensional flow in an infinite domain by tracing out approximate solution curves in three-dimensional phase space using the shooting method. This is one of the few instances where an exact solution has been obtained for the nine-velocity gas. Comparison to the shock structure in a monatomic perfect gas, as given by the Navier-Stokes equation, shows excellent agreement. The shock in the nine-velocity gas, has an overshoot in entropy like in a monatomic gas. The near-equilibrium flow technique for discrete-velocity gases (see above), a kinetic flux-splitting method based on the local thermodynamic equilibrium, is also seen to capture the shock structure at the level of the finite-difference discretization (cell size) remarkably well.

5. 2-D Adiabatic Channel Flow by Direct Simulation with a Lattice Gas

The viscous and compressible but laminar flow of a perfect gas through an adiabatic channel is not a fully understood problem. Its incompressible counterpart constitutes Hagen-Poiseuille flow and is an exact solution of the Navier-Stokes equations. There have been few instances of a full simulation of the problem of laminar compressible viscous channel flow. One of the problems is the imposition of the downstream boundary conditions. In this section, a simulation of the channel flow using the nine-velocity model is described. The lattice gas method being a particle method, the imposition of the boundary conditions is simpler.

The computational domain is rectangular. The interaction of the system with the external surroundings is only through the perimeter of the domain. With flow along the longer dimension, the interactions along the shorter sides constitute the inflow-outflow boundary conditions and the interactions along the longer dimensions describe what happens on the channel walls.

The simulation of the wall boundary condition is simple. Two possible wall collisions are: i) specular reflection; only the component of velocity perpendicular to the wall is reversed. In this case, the accommodation coefficient of the wall is zero, *i.e.*, flow properties parallel to the wall are unaffected by the wall. The flow velocity at the wall can be non-zero. ii) "bounce-back"; the velocity of the particle impinging the wall is reversed. The accommodation coefficient in this case is two. This is a rather severe case of a wall from which the particles do not bounce in random directions, but instead remember their incoming velocity and reverse it on collision. A realistic wall has an accommodation coefficient of unity (diffuse wall) and this is easily achieved by uniformly but randomly choosing between the two types of reflection. In both the specular and bounce-back reflection of particles at the wall, the particle speeds are preserved, ensuring adiabaticity of the wall.

The inflow boundary condition is implemented through a "reservoir," a body of fluid which is unaffected by the flow in the channel. The reservoir in the present case is a small, independent and steady state constantly updated region, periodic in the flow direction, located upstream of the actual channel. A particular lattice column of the reservoir is assumed to be located immediately upstream of the channel entrance, so

that particles at this lattice column directed downstream are introduced at the channel entrance during the following time step. In the computations presented here, the upstream reservoir uses a mobius-strip boundary condition for the walls parallel to the flow, and a periodic boundary condition in the flow direction, as introduced by Kadanoff *et al.* in 1989. The flow in the upstream reservoir is sustained by imposing a body force, the level of which is adjusted to obtain the required flow rate. This generates a velocity profile which is parabolic for low forcing levels.

The out flow boundary condition at the downstream end of the computational channel amounts to the imposition of a downstream pressure at the last column of lattice sites. That column is modeled as a porous wall with the porosity depending inversely on the downstream pressure to be simulated. For a given pressure, the porosity of the wall at any time is uniform across the wall, but changes location at each time step to preclude the formation of any upstream patterns.

The multi-computer is configured as a linear array of processors along the flow direction. The computational domain is equally partitioned along the flow direction and the partitions assigned to the nodes (one computer of the multi-computer). There are no regions of overlap among the various nodes and the inter-node communication is limited to moving particles either leaving or entering the domain of a node. All the computations presented here were done with the Intel iPSC/860 GAMMA parallel machine, which consists of 64 nodes of iPSC/860 wired in a hypercube architecture. The communications in the present case were handled under the Reactive Kernel environment of Seitz *et al.*. The sustained lattice site update rate for these computations, with the present implementation, was about one million sites per second.

Noteworthy features of the results are:

- The flow accelerates slowly at first, but much more rapidly at higher velocities. The last 50% of the increase in velocity is over about 12 widths of the channel (the full channel is 128 widths long).
- The velocity profile, initially parabolic, flattens near the downstream end.
- The pressure profile across the channel is quite flat up to relatively high flow velocities.
- The flow is nearly isothermal (width-averaged temperature almost constant in the downstream direction) at low velocities, rather than constant density, as might have been expected.
- The width-averaged pressure drops off nearly linearly down the channel at low velocities, becoming increasingly non-linear at higher velocities.
- The width-averaged density and pressure profiles are very similar at low velocities.
- The effects of viscous dissipation are confined to a region near the walls. A rise in entropy observed in the central core is mainly due to the falling density.

6. Publications

1. Goldstein, D. and Sturtevant, B. 1989 Discrete Velocity Gasdynamics Simulations in a Parallel Processing Environment, AIAA-89-1668, AIAA 24th Thermophysics Conf., Buffalo, NY.
2. Goldstein, D., Sturtevant, B. and Broadwell, J. E. 1989 Investigations of the Motion of Discrete-Velocity Gases, in "Rarefied Gasdynamics: Theoretical and Computational Techniques," *Progress in Astronautics and Aeronautics*, Vol. 118, Muntz, E. P., Weaver, D. P., and Campbell, D. H., 100, AIAA, Washington, D. C..

3. Goldstein, D. 1990 Investigations of a Discrete Velocity Gas, Ph.D. Thesis, Aeronautics, California Institute of Technology, Pasadena, CA.
4. Goldstein, D. 1990 Near-Continuum Applications of a Discrete-Velocity Gas Model, Proceedings of 17th Intl. Symp. on Rarefied Gasdynamics, VCH Verlagsgesellschaft, Weinheim, Germany.
5. Goldstein, D. 1990 Discrete-velocity collision dynamics for polyatomic molecules, LANL Report LA-UR 90-3243, Los Alams, NM, (to be published, Phys. Fluids A, 4, 1992).
6. Goldstein, D. 1990
7. Inamuro, T. and Sturtevant, B. 1990 Numerical Study of discrete-velocity gases, Phys. Fluids A 2, 2196.
8. Inamuro, T. and Sturtevant, B. 1990 Heat Transfer in a Discrete-Velocity Gas, Proceedings of 17th Intl. Symp. on Rarefied Gasdynamics, VCH Verlagsgesellschaft, Weinheim, Germany.
9. Nadiga, B. T., Broadwell, J. E. and Sturtevant, B. 1989 Study of a Multi-Speed Cellular Automaton, in "Rarefied Gasdynamics: Theoretical and Computational Techniques," *Progress in Astronautics and Aeronautics*, Vol. 118, eds. Muntz, E. P., Weaver, D. P., and Campbell, D. H., 155, AIAA, Washington, D. C..
10. Nadiga, B. 1992 A Study of Multi-Speed Discrete Velocity Gases, Caltech Ph.D. Thesis, Pasadena, CA.

7. Participating Personnel and Degrees Earned

Name	Title	Degree	Date	Thesis Title
Bradford Sturtevant	Professor of Aeronautics			
James E. Broadwell	Research Associate			
David Goldstein	Graduate Research Assistant	Ph.D.	6/90	Investigations of a Discrete Velocity Gas
	Post Doctoral Fellow			
Balu Nadiga	Graduate Research Assistant	Ph.D.	6/92	A Study of Multi-Speed Discrete Velocity Gases

8. Interactions

Extensive interaction was had with scientists at the Los Alamos National Laboratory and the Center for Nonlinear Studies, LANL, through participation in the following:

1. NATO Advanced Research Workshop on Lattice Gas Methods for Partial Differential Equations; Theory Applications and Hardware
2. Workshop on Cellular Automata: Theory and Experiment

3. Summer Student Fellowship, September 1989 (B. Nadiga)
4. Postdoctoral Fellowship at LANL, August 1990 (D. Goldstein).
5. Collaboration visit to LANL, September 1990 (B. Nadiga)
6. Winter School on Complex Systems, Tucson, AZ, January 1992.

Our group is a participant in the NSF National Center for Research in Parallel Computing (CRPC), a consortium of Rice University, California Institute of Technology, Argonne National Laboratory, Los Alamos National Laboratory University of Tennessee, and Syracuse University. Through seminars and workshops we have had contact with scientists at all of those institutions.