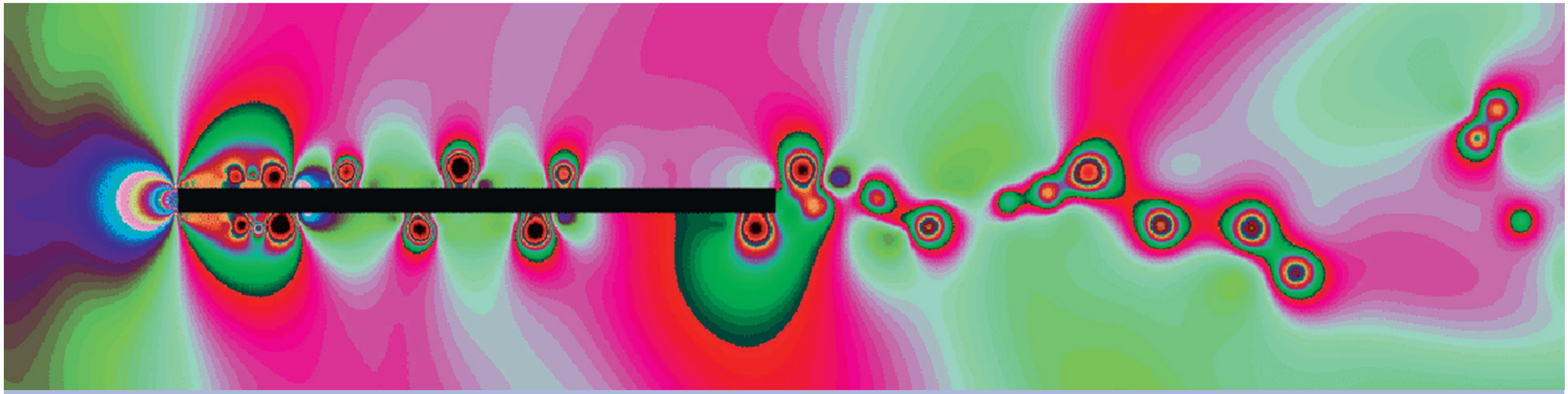


Lattice-Boltzmann
a versatile tool for multiphase

Fluid Dynamics
and other complicated flows

Shiyi Chen, Gary D. Doolen, and Kenneth G. Eggert

Long-term research efforts at the Laboratory often produce results that prove highly valuable to U.S. industry. The example described here is a new approach to modeling the flow of multiphase fluid mixtures, such as oil and water, through very complicated geometries. This new modeling technique, called the lattice-Boltzmann method, evolved out of ideas that have been intensely investigated since 1985, when Laboratory scientists and others discovered that very simple models of discrete particles confined to a lattice can be used to solve very complicated flow problems.

This lattice method can be regarded as one of the simplest microscopic, or particle, approaches to modeling macroscopic dynamics. It is based on the Boltzmann transport equation for the time rate of change of the particle distribution function in a particular state. The Boltzmann equation simply says that the rate of change is the number of particles scattered into that state minus the number scattered out of that state.

The method is fully parallel (the same calculations are performed at every lattice site) and local (only nearby particles interact with each other). It is therefore easily programmed and runs efficiently on parallel machines. Complex boundary conditions are incorporated in a straightforward way and cause the calculational speed to decrease by only a few percent. The method yields a good approximation to the standard equations of fluid flow, the Navier-Stokes equations, in the limit of long wavelengths and low frequencies. Also, recent generalizations of the method have extended its applicability to multiphase flows, chemically reacting flows, diffusion and thermohydrodynamics.

United States oil companies have expressed considerable interest in the lattice-Boltzmann method for addressing problems in oil recovery. For example, we are collaborating with the Mobil Exploration and Producing Technical Center on using the lattice-Boltzmann method to simulate the flow of oil and water through oil-bearing sandstone at a scale and an accuracy never before possible. Mobil provided Los Alamos with 5-micron-resolution sandstone geometries for use in the simulations. (Typical pore diameters are tens of microns.) The goal of the work is to simulate, at the scale of individual pores in the rock, what happens when water is pumped though the rock to force out oil. Viscosities, surface tensions, contact angles, and surfactant effects can be varied to determine how well this method of oil recovery can be made to work in specific circumstances. The collaboration is described by Mobil and Los Alamos scientists in the companion article, "Toward Improved Prediction of Reservoir Flow Performance—Simulating Oil and Water Flows at the Pore Scale." The work has included the development of software to calculate relative permeabilities of oil and water in complex geometries. The software received an R&D-100 award for 1993.

The lattice-Boltzmann work is a superb example of applying the extraordinary computer power and expertise in computational physics available at Los Alamos to problems in petroleum production. The Laboratory's success at projects of this type helped motivate the oil companies to ask that Congress substantially increase DOE support for oil and gas research and make those funds available for significant new collaborations between the oil and gas industry and the National Laboratories. The result is ACTI—the Advanced Computational Technology Initiative—an initiative that will receive $30–50 million in funding in 1995.

In this article we will first sketch the basic ideas of the lattice-Boltzmann method and its general applicability. We will then explain how the lattice-gas and lattice-Boltzmann methods are adapted to describe the dynamics at the interfaces between two immiscible fluids such as oil and water and present some simulations of phase separation. Finally, we will mention a few of the new directions into which lattice-Boltzmann research is moving. Specific applications to the flows in oil reservoirs are discussed in the companion article.

Illustration on previous spread: A lattice-Boltzmann simulation of flow past a slab shows the complicated flow patterns that can be modeled with this technique. The lattice is 1024 × 256 sites; the thickness of the slab is 32 sites, which gives the flow a Reynolds number of 960. Wind-tunnel boundary conditions are used—the flow velocity at the entrance (left), the top, and the bottom boundaries is fixed. The top image shows contours of equal vorticity; the bottom image shows the pressure distribution of the flow. The simulation was done using the Connection Machine 2 at the Advanced Computing Laboratory.

Lattice Methods for Modeling Continuum Dynamics

Lattice methods, including the lattice-gas method and its derivative, the lattice-Boltzmann method, present powerful alternatives to the standard "top-down" and "bottom-up" approaches to modeling the behavior of physical systems. The "top-down" approach begins with a continuum description of macroscopic phenomena provided by partial differential equations. The Navier-Stokes equations for incompressible fluid flows are an example. Numerical techniques, such as finite-difference and finite-element methods, are then used to transform the continuum description into a discrete one in order to solve the equations numerically on a computer.

The "bottom-up" approach is based on the microscopic, particle description

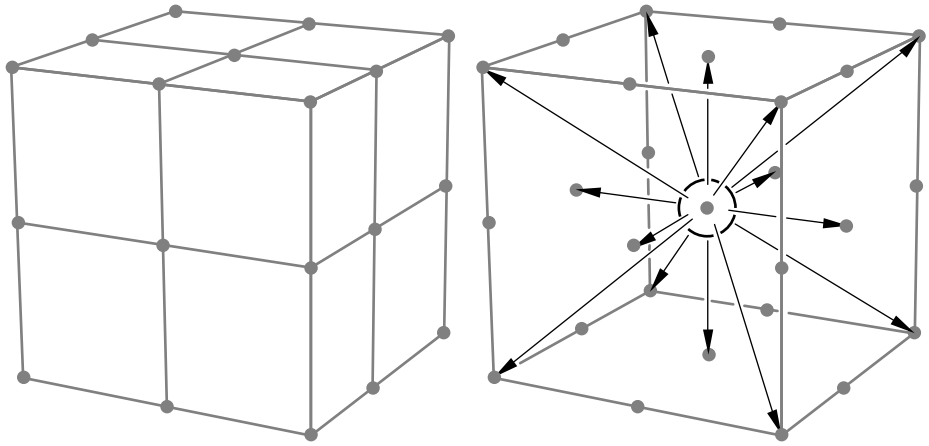


Figure 1. Allowed Velocities at a Lattice Site

The arrows indicate the magnitudes and directions of the allowed velocities e_i at a lattice site in a three-dimensional lattice-Boltzmann simulation. The lattice has a cubic structure. Six arrows point to nearest-neighbor sites. Eight arrows point along body diagonals. The sphere at the lattice site represents zero velocity, $e_0 = 0$. Lattice-Boltzmann simulations based on a proper equilibrium particle distribution and this minimum set of velocities preserve the desired isotropy of fluid properties.

provided by the equations of molecular dynamics; here the position and velocity of each atom or molecule in the system are closely followed by solving Newton's equations of motion. This microscopic description is straightforward to program on a computer but simulations using the largest computers presently available are limited to very small systems (ten million particles) and very short times (a few picoseconds). Therefore molecular dynamics simulations are more suitable for understanding the fundamental interactions that underlie macroscopic material properties than for modeling macroscopic dynamics.

Intermediate between the two schemes are the lattice-Boltzmann and lattice-gas methods, which might be considered mesoscopic approaches. The lattice methods begin from a particle description of matter: A gas of particles exists on a set of discrete points that are spaced at regular intervals to form a lattice. Time is also divided into discrete timesteps, and during each timestep particles jump to the next lattice site and then scatter according to simple kinetic rules that conserve mass, momentum, and energy. This simplified molecular dynamics is very carefully crafted to include the essentials of the real microscopic processes. Consequently the macroscopic, or averaged, properties of lattice simulations obey, to a good approximation, the desired continuum equations. Despite their origin in a particle description, lattice methods are essentially numerical schemes for studying averaged macroscopic behavior. They nevertheless retain the advantages of a particle description, including clear physical insight, easy implementation of boundary conditions, and fully parallel algorithms.

Because lattice methods are entirely local, they are extremely fast. A simulation of a simple lattice-gas model can attain a speed of 20 gigaflops on a 512-processor CM-5 Connection Machine. Typical simulations of flow through porous media include 100 million lattice sites and run for 5000 timesteps and therefore require only a few hours on that machine. When applied to periodic geometries, the three-dimensional lattice-Boltzmann model is able to achieve the same spatial resolution as conventional methods in half the time. Also, because boundary conditions—even complex ones—are imposed locally, lattice methods simulate flows in both simple and complex geometries with almost the same speed and efficiency. They are therefore suitable for simulating flows in the extremely complex geometries of porous media whereas conventional methods are not. Finally, developing code for lattice methods is considerably faster and easier than for traditional schemes.

General lattice models already exist for solving the equations of fluid flow, the wave equation, and the diffusion equation. Special versions of these models have been developed for simulating flow through porous media, turbulent flows, phase transitions, multiphase flows, chemically reacting flows, thermohydrodynamics, magnetohydrodynamics, the dynamics of liquid crystals and the design of semiconductors. These models are validated by precise comparisons with other numerical algorithms, analytic results, and experiments.

The Lattice-Boltzmann Method

In the lattice-Boltzmann method, space is divided into a regular lattice (for example, a simple cubic lattice) and real numbers at each lattice site represent the single-particle distribution function at that site, which is equal to the expected number of identical particles in each of the available particle states *i*. In the simplest model, each particle state *i* is defined by a particle velocity, which is limited to a discrete set of allowed velocities. During each discrete timestep of the simulation, particles move, or hop, to the nearest lattice site along their direction of motion, where they "collide" with other particles that arrive at the same site. The outcome of the collision is determined by solving the kinetic (Boltzmann) equation for the new particle-distribution function at that site and the particle

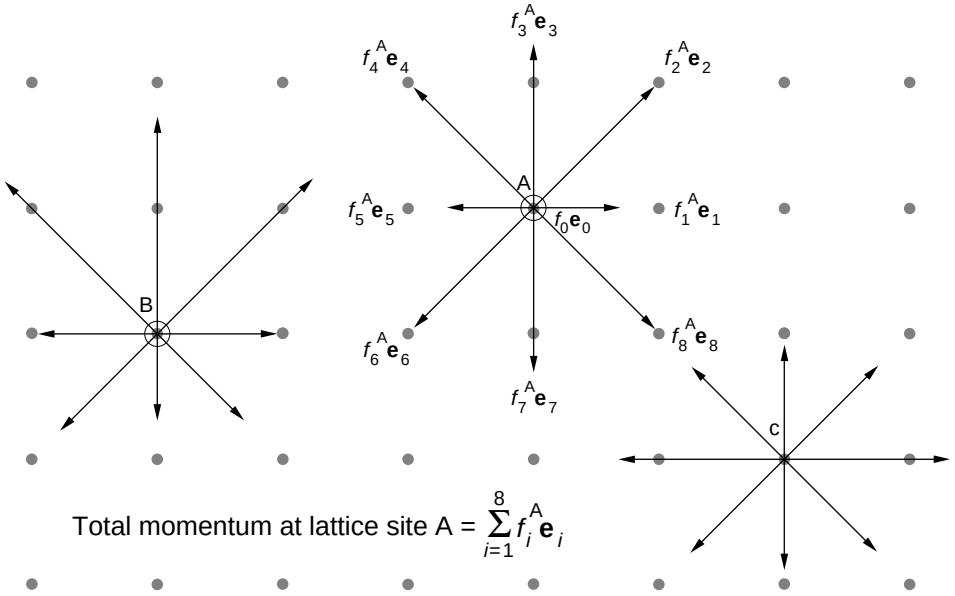


Figure 2. Momentum Distributions in Two Dimensions

The single-particle distribution function at each lattice site, $f_i(\mathbf{x},t)$, equals the expected number of identical particles in each of the available particle states *i*. Particle velocities $\mathbf{e}_i$ are limited to a discrete set defined by the geometry of the lattice, and the momentum distribution at a lattice site is equal to $f_i(\mathbf{x},t)\mathbf{e}_i$. On a two-dimensional square lattice, eight directions of motion are possible, so $i = 0, 1,\ldots, 8$. Each arrow indicates the momentum in one of the allowed directions of motion. The circles represent the rest particles. The figure shows several examples of momentum distributions in two dimensions. The distribution at site B has a net momentum in direction 3. The net momentum is equal to zero at sites A and C.

distribution function is updated.

More specifically, the single-particle distribution function at a single site in a simple cubic lattice is represented by a set of real numbers, $f_i(\mathbf{x},t)$,the expected number of particles at lattice site $\mathbf{x}$ and time t moving along the lattice vector $\mathbf{e}_i$, where each value of the index i specifies one of the allowed directions of motion. Figure 1 shows these directions. Six lattice vectors point to the six nearest-neighbor sites. Eight lattice vectors point along the body diagonals to the next sites along those diagonals. Thus particles can travel in fourteen directions from each lattice site. The ball in the center denotes the vector $\mathbf{e}_0$,which is equal to 0 and represents particles that are not moving. In total, fifteen real numbers describe the particle distribution function at a site.

The first operation in each timestep Δt of the calculation is to advance the particles to the next lattice site along their directions of motion. Since speed equals the distance traveled divided by Δt, this model has only three speeds, zero for particles at rest, c for particles moving to nearest-neighbor sites and $\sqrt{3}c$ for particles moving to the next sites along body diagonals. Usually the units are chosen such that the distance to nearest neighbors and Δt are unity, so that $c = 1$ and the lattice vector $\mathbf{e}_i$ is numerically equal to the velocity of the particles moving in direction i. If we also set the mass of each particle equal to unity, the momentum in direction i at site $\mathbf{x}$ and time t is just $f_i(\mathbf{x},t)\ \mathbf{e}_i$. Figure 2 illustrates sample momentum distributions in two dimensions.

The second operation is to simulate particle collisions, which cause the particles at each lattice site to scatter into different directions . The collision rules are chosen to leave the sum of the f_i's unchanged. (No particles are lost.) The rules are also selected to conserve the total energy and momentum at each lattice site. To ensure that the particles have zero average velocity at boundaries (both perpendicular and parallel to the walls), one normally imposes "bounce-back" boundary conditions: Any flux of particles that hits a boundary simply reverses its velocity so that the average velocity at the boundary is automatically zero, as observed experimentally.

The outcome of collisions is very simply approximated by assuming that the momenta of the interacting particles will be redistributed at some constant rate toward an equilibrium distribution f_i^{eq}. This simplification is called the single-time-relaxation approximation. In mathematical terms, the time evolution of the single-particle distribution is given by

$$f_i(\mathbf{x} + \mathbf{e}_i,\ t + 1) = f_i(\mathbf{x},t) - \frac{f_i(\mathbf{x},t) - f_i^{\mathrm{eq}}(\mathbf{x},t)}{\tau},$$

where $i = 0, 1,\ldots, 14$. The second term on the right-hand side is the simplified collision operator Ω_i. The rate of change toward equilibrium is $1/\tau$, the inverse of the relaxation time, and is chosen to produce the desired value of the fluid viscosity.

Figure 3 illustrates the single-time-relaxation approximation in two dimensions. The net momentum of the incoming state is zero. In that case, if no external forces exist, the equilibrium distribution consists simply of equal amounts of particle momentum in each of the allowed directions of motion. The collision rules will therefore force the larger f_i's at the site to decrease and the smaller f_i's to increase so that the particle distribution is closer to the equilibrium distribution after the collision than before. External forces (grav-

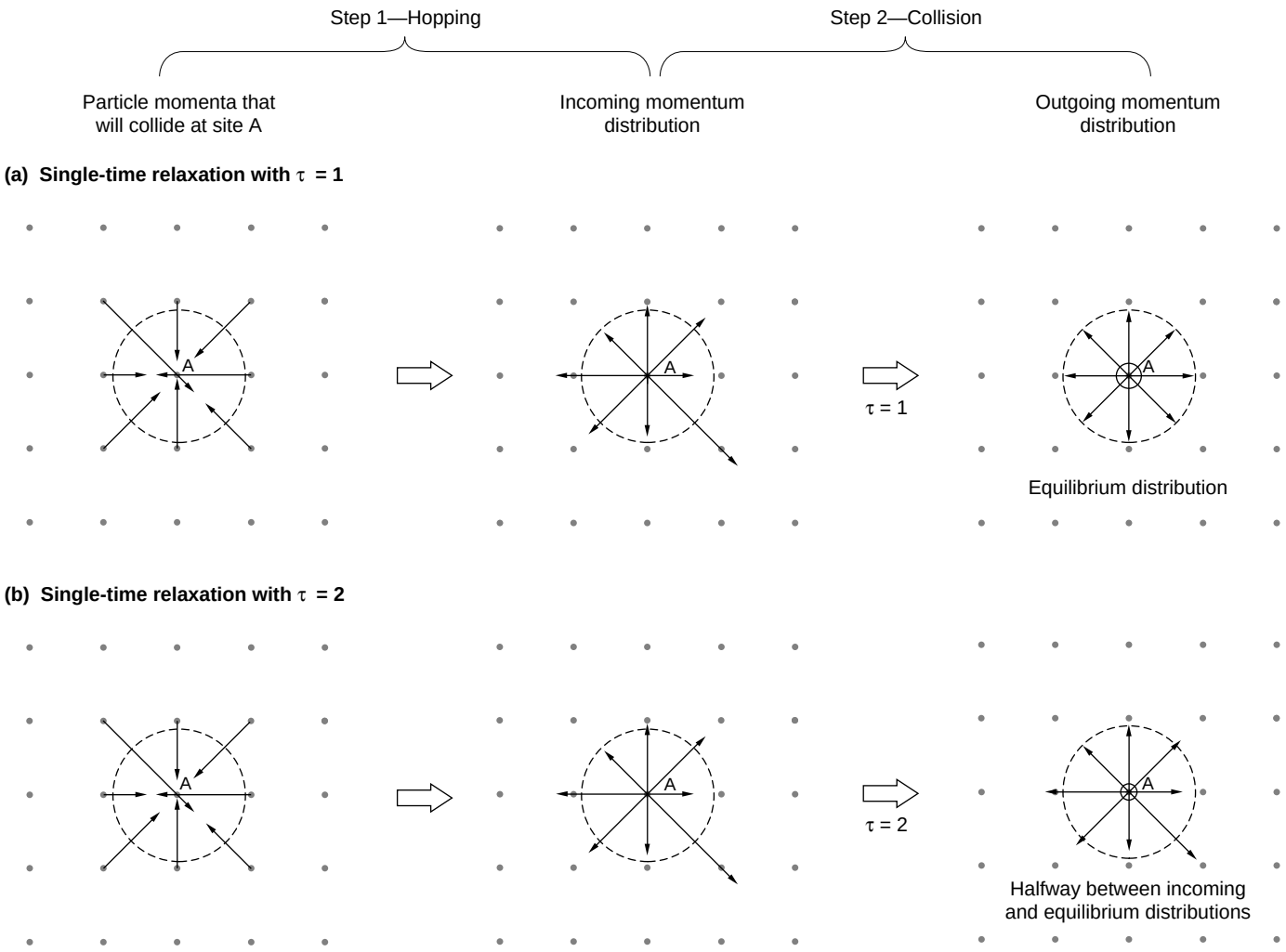


Figure 3. The Single-Time-Relaxation Process

In the single-time-relaxation approximation, the momentum distribution at each lattice site is forced toward the equilibrium distribution at each timestep. In the absence of external forces, the equilibrium distribution of a state with zero net momentum is just equal amounts of momentum in each direction. The figure illustrates the two calculational steps that occur during each timestep. First the incoming momentum distribution assembles at a lattice site as particles at the neighboring sites hop along their directions of motion to that site. Second, the incoming distribution changes, according to the single-time-relaxation collision rule, to an outgoing distribution that is closer to the equilibrium distribution. When $\tau = 1$, the incoming momentum distribution changes to the equilibrium distribution in one time step; when $\tau = 2$, the outgoing momentum distribution is halfway between the incoming and the equilibrium distributions.

ity or electromagnetic forces) can be added to the model and make the f_i's grow in the direction of the net force and shrink in the opposite direction.

Although lattice models consist of a very simple set of rules, those rules lead to very complicated flow patterns. The opening pages of this article show a snapshot from a two-dimensional lattice-Boltzmann simulation performed by Lishi Luo here at the Laboratory. The simulation models the flow of air past a rectangular plate. Periodic boundary conditions are imposed perpendicular to the plate; wind-tunnel boundary conditions (air flowing in from the left at higher pressure and out at the right at lower pressure) are imposed in the flow direction. Attached vortices and vortex shedding are evident, showing the complicated flow patterns that can be modeled with lattice-Boltzmann methods. Detailed, quantitative comparisons with other methods and with experiment have verified the accuracy of this method. In general, lattice-Boltzmann simulations agree with exact solutions to the Navier-Stokes equations to second order in the lattice spacing and the timestep.

The lattice-Boltzmann method is an outgrowth of lattice-gas models, providing something akin to an ensemble average of many realizations of a lattice gas but without the unphysical effects.

Lattice-gas models differ from lattice-Boltzmann models in that the former follow the motion of actual particles whereas the latter utilize the expected values of the particle-distribution function. The gas is composed of identical particles that obey an exclusion principle: At most one particle can occupy a given particle state at a given time. Since $N_i(\mathbf{x},t)$, the number of particles that occupy state i at a lattice site, is either 0 or 1, only single-digit binary arithmetic is required to update the particle numbers following each collision. Consequently lattice-gas calculations are extremely fast. Collision rules specify the possible outcomes of two-particle and three-particle collisions and the explicit choice at each site is implemented by random sampling. The lattice gas is therefore very noisy, and spatial and temporal averaging are required to obtain macroscopic quantities. Also the method has several major drawbacks, including restriction to low Reynolds number, lack of Galilean invariance (convective flow velocities don't add properly unless the system is at nearly constant density), and an unphysical equation of state in which the pressure depends on the local velocity in addition to the usual dependence on the local density.

In contrast, the lattice-Boltzmann method uses real (continuous) numbers to describe a particle distribution at each site; in this sense it approaches a continuum description. Although one pays a penalty in that floating-point arithmetic operations are now required to carry out the simulations, the continuum feature eliminates most of the noise associated with lattice-gas simulations. In addition, the local equilibrium particle distribution f_i^{eq} that appears in the collision operator can be chosen to eliminate the unphysical features of the lattice gas while including dependence on the local fluid variables only and leading to the appropriate macroscopic equations. In other words, although lattice-Boltzmann simulations ignore particle-particle correlations and use simplified collision rules, the collision rules can be tailored to reproduce the correct evolution of the macroscopic behavior of a system in a wide variety of circumstances. The relevant equations are presented in the sidebar, "Equations of the Lattice-Boltzmann Method."

Strategies for Modeling the Flow of Two Fluid Phases

Modeling the flow of two immiscible fluids, such as oil and water, presents the difficulty of how to treat the dynamics at the interfaces between the two. These dynamics control phenomena such as the flow of oil and water through porous media, the development of viscous fingering, which occurs when water pushes oil, and dendrite formation (such as the growth of snowflakes). Traditional finite-difference and finite-element schemes can be used to model two-phase flow in simple flow geometries, but they are difficult to apply in the complicated geometries of porous media. Here we describe lattice methods for complex two-phase phenomena; these methods are being successfully applied to problems in oil recovery.

To extend lattice methods to the flow of two immiscible fluids (say red and blue fluids), one must double the information at each lattice site. In the lattice-Boltzmann approach this is done by postulating a single-particle distribution for each of the fluids. It is also necessary to create new scattering rules that will cause the two fluids to separate at an interface and to emulate the effects of surface tension. The essential idea is to compute a force at each lattice site that depends on, say, the red-fluid density at the neighboring sites and that pushes the red fluid in the direction of increasing red-fluid density. The effect of the force must be added to the collision operator in such a way that it does not change the total momentum of the two fluids. The size of the force must be chosen to produce the desired surface tension between the two fluids. Under these rules, an initially random mixture of the red and blue fluids should unmix and form an equilibrium distribution in which a spherical interface separates the two fluids, as expected physically in mixtures of oil and water.

Lattice-gas simulations of immiscible fluids. The extension of lattice methods to two immiscible fluids was done originally in the context of lattice gases. Our particular method implements the effects of surface tension in a purely local manner—through the introduction of two species of colored holes. A hole acts like a massless "ghost" particle that moves freely on the lattice but carries no momentum. A hole of one color is created at a lattice site when an incoming particle of that color is scattered into a new direction; the new hole moves in the incoming direction of the scattered particle and thereby carries a memory of that particle. The hole is annihilated, or disappears, when it meets a particle of the same color traveling in the same direction.

To create surface tension, a new collision rule is added to the usual ones that causes the colored particles at a site to respond to the presence of colored holes by moving in the opposite direction. The overall effect is like that of a short-range attractive potential among particles of the same color. Although the "color potential" has a range of more than one lattice spacing, only local information is needed to compute the results of collision at each lattice

site; consequently the colored-hole scheme is much faster for modeling the effects of surface tension than methods requiring the calculation of nearest-neighbor color gradients.

The colored-hole scheme has been used successfully to simulate phase separation, surface tension between phases, and contact angles between fluids and solid walls. Figure 4 shows the results of a lattice-gas simulation of red and blue fluids: Red drops have formed in blue fluid starting from a random initial configuration in which the density of red particles was equal to one-fifth the density of blue particles. Figure 5 demonstrates that the results shown in Figure 4 obey the Laplace formula for surface tension. That is, the pressure drop Δp across the boundary of each drop is given by

$$\Delta p = p_{\text{red}} - p_{\text{blue}} = \frac{\sigma}{R},$$

where p_{red} is the pressure of red particles inside the drop, p_{blue} is the pressure of blue particles outside the drop, σ is the surface-tension coefficient, and R is the radius of the drop. Figure 5a shows the pressure versus the distance r from the center of a drop; the pressure change at the red-blue interface demonstrates the existence of surface tension. Figure 5b shows Δp, the pressure change across the interface of the drop for drops of different radii R. As required by the Laplace formula, the pressure change is directly proportional to $1/R$.

In addition to surface tension at fluid-fluid interfaces, the two-fluid lattice-gas model must also simulate interactions between the fluids and the walls. Typically, when the interface between two fluids intersects a solid wall, the angle of intersection is fixed. Figure 6 illustrates the two contact angles, one for each fluid, formed at the point of intersection. By definition, the sum of the two contact angles is equal to 180°.

The contact angle of a fluid decreases as the affinity, or preference, of the wall for that fluid increases. That preference is called wettability. On a strongly water-wet surface, water droplets in a background of oil will tend to spread out on the surface and the contact angle of water will be close to 0°. On a strongly oil-wet surface, those water droplets will bead up and the contact angle will be close to 180°. In our lattice-gas simulations, wettability is controlled by a special rule for collisions of colored holes with the wall: With a certain probability P, a hole of either color bounces back and becomes, say, a red hole. This rule can produce contact angles for the red fluid of between 20° and 180°.

Figure 7 shows the results of colored-hole two-fluid simulations in which different values of the probability P for the upper and lower surfaces of a wall (white) have led to marked differences in the contact angles of the red fluid. The results shown were obtained by averaging 12 realizations of the lattice gas.

Lattice-Boltzmann model for two fluids. Lattice-gas simulations produce realistic surface phenomena for immiscible fluids, but they do so only when temporal and spatial averaging are used to eliminate the noise induced by particle fluctuations. A more convenient approach is to extend the lattice-Boltzmann method to colored fluids and use color gradients, or nearest-neighbor interactions, for modeling interfacial dynamics. In this approach, each colored fluid is described by a single-particle distribution function, and each is assigned a number density as well as a characteristic relaxation time, which

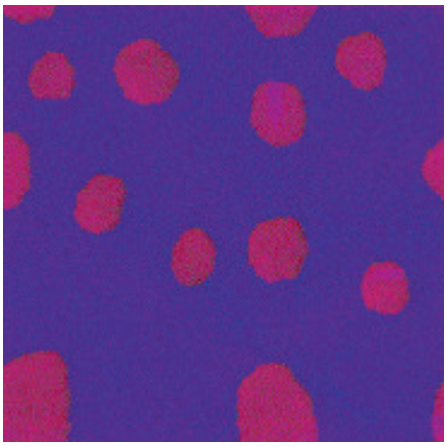


Figure 4. Droplet Formation in Two-Phase Lattice-Gas Mixtures

The figure shows the results of a lattice-gas simulation in which the dynamics of the interface between red and blue phases was modeled by using the colored-hole scheme summarized in the text. The simulation produced this distribution of red droplets in a blue background after 17,200 time steps, starting from a random initial distribution of red and blue particles on 512 × 512 lattice sites. The total particle density is 0.4 and the ratio of red to blue particles is 1/5. Because the lattice gas is very noisy, the droplets have very rough surfaces, in contrast to the smooth surfaces expected at fluid-fluid interfaces. Consequently the results of the lattice-gas simulations must be averaged spatially and temporally to be compared with the macroscopic description of immiscible fluids (see Figure 5). This figure should also be compared with Figure 8, which shows that the lattice-Boltzmann method produces smoother, more realistic droplets.

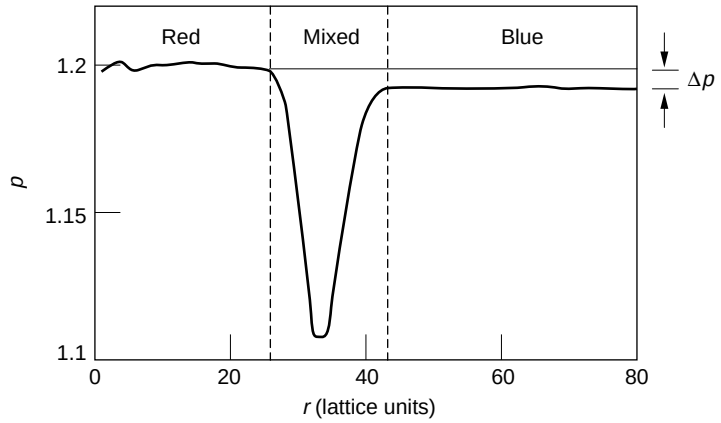
Figure 5. Verification of the Laplace Formula for Surface Tension in Two-Phase Lattice-Gas Simulations

For real droplets in a mixture of immiscible fluids, a pressure difference across the interface balances the surface tension created by the mutual attraction of particles of like kind. The relation is given by the Laplace formula, $\Delta p = \sigma/R$ where σ is the surface-tension coefficient and R is the radius of the droplet. To compare the lattice-gas results of Figure 4 with that macroscopic description, the pressure is calculated from the local particle-number density, $p = n/3$, and the results are averaged temporally over 1000 timesteps and spatially in the circumferential direction around the center of each droplet.

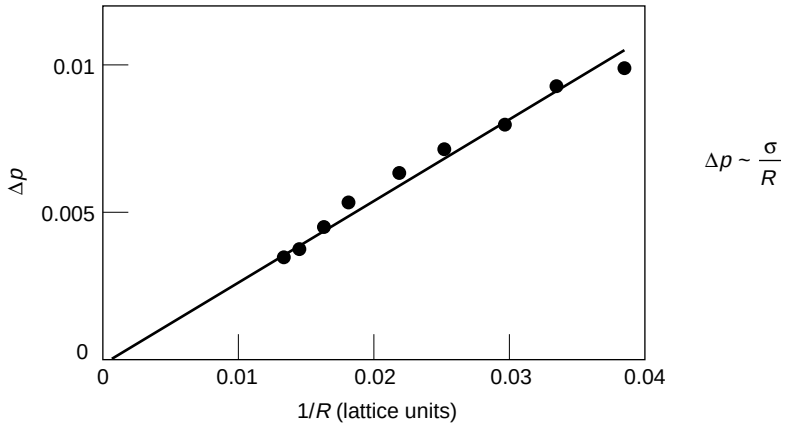
(a) That average pressure is plotted as a function of the distance r from the center of a droplet. The pressure difference between the red phase and the blue phase demonstrates the existence of surface tension in these two-phase simulations.

(b) The pressure difference across the droplet surface is plotted as a function of $1/R$, where R is the radius of the droplet. The linear relation shows that the surface tension coefficient σ is a constant, as required by the Laplace formula. Thus the averaged results of the colored-hole, two-phase lattice-gas simulations reproduce the correct macroscopic interfacial dynamics.

(a) Pressure profile of red droplet



(b) Pressure difference across red-blue interface for red droplets of different radii (R)



determines its viscosity. The collision operator now has two parts. The first part of Ω_i induces single-time relaxation to equilibrium, as was done for the single phase. Again each fluid tends to relax to a local equilibrium distribution that depends on the local density and velocity and is analogous to the single-phase equilibrium distribution presented in the sidebar. The mass of each fluid is conserved and the total momentum of the system is conserved.

The second part of the collision operator Ω_i depends on the red and blue densities at nearest neighbors and determines the dynamics at the fluid-fluid interfaces. It is given by

$$\frac{A_k}{2} \left| \mathbf{F} \right| \left[\frac{(\mathbf{e}_i \cdot \mathbf{F})^2}{\left| \mathbf{F} \right|^2} - 1/2 \right],$$

where k denotes red or blue, A_k is a free parameter that controls the surface tension, and $\mathbf{F}$ is the local color gradient, defined as

$$\mathbf{F}(\mathbf{x}) = \sum_i \mathbf{e}_i \, [\rho_r(\mathbf{x} + \mathbf{e}_i) - \rho_b(\mathbf{x} + \mathbf{e}_i)].$$

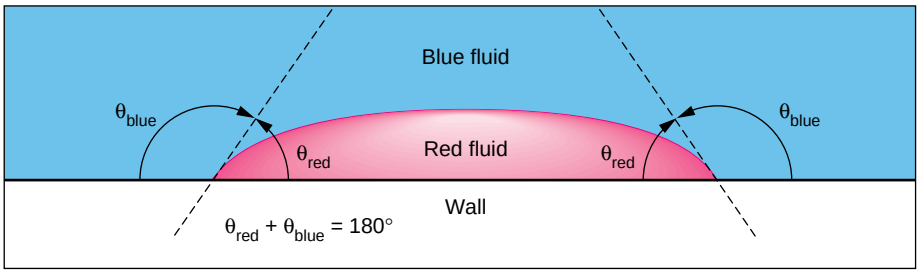


Figure 6 . The Definition of Contact Angle

The contact angle is defined as the angle between a two-fluid interface and a solid surface. As shown in the figure, each fluid has its own contact angle and the sum of the two must equal 180°. The wetting fluid (the fluid that tends to wet the surface) has a contact angle of less than 90°, and the nonwetting fluid (the fluid that has less affinity for the solid surface) has a contact angle of greater than 90°.

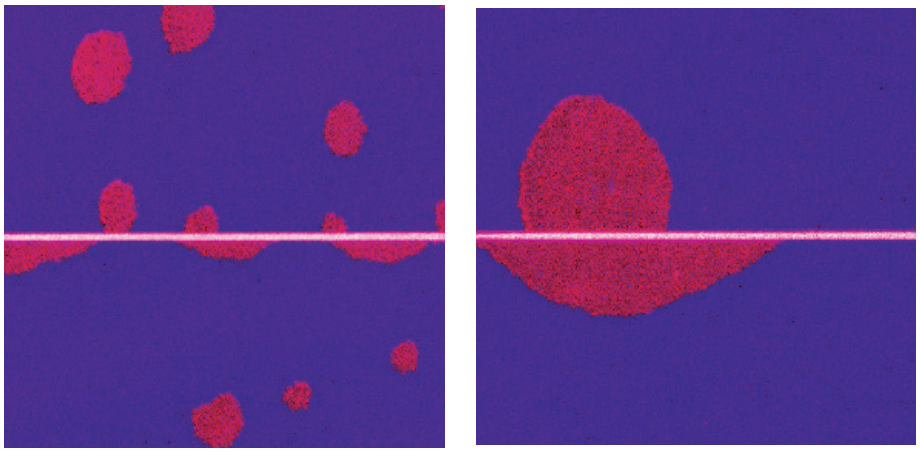


Figure 7. Contact Angles in Two-Phase Lattice-Gas Simulations

This simulation demonstrates the ability of lattice-gas simulations to model different contact angles, or different wettability conditions, as required in studies of porous-media flow. The simulation conditions are identical to those described in Figure 4 except that a solid horizontal wall (white) divides the computational box into an upper and a lower region. The upper surface of the wall has a greater affinity for the blue fluid than for the red fluid, whereas the opposite is true of the lower surface of the wall. The affinity, or preference, of the wall for one fluid over the other is modeled by a special rule for collisions between a hole and the wall that controls the color of the hole flux at the walls. The rule specifies that when a hole of either color collides with a wall, there is a probability *P* that it will bounce back and become a red hole. In the simulation shown the upper surface has *P* = 0.2; that choice produces a surface that is strongly blue-wet, and the contact angle of the red fluid is greater than 90°. The lower surface has *P* = 0.8, which results in a strongly red-wet surface and a contact angle for the red fluid of close to 0°.

In the incompressible limit, the density in a single-phase region is uniform and therefore the local color gradient is zero. Thus this second part of the collision operator does not contribute. In a mixed-phase region, this part of the collision operator maintains the interfaces between fluids by forcing the momentum of the red fluid, $\mathbf{j}^r = \Sigma_i f_i^r \mathbf{e}_i$, to align with the direction of the local color gradient. In other words, the red density at an interface is redistributed to maximize the quantity $-(\mathbf{j}\cdot\mathbf{F})$. The blue-particle distribution can then be obtained by applying mass conservation along each direction: $f_i^b = f_i - f_i^r$.

Using a scaling and expansion procedure similar to that used to derive the macroscopic behavior of a single phase (see sidebar), one can rigorously prove that each fluid will obey the Navier-Stokes equations and that the pressure difference across fluid-fluid interfaces will obey the Laplace formula. Results of two-phase lattice-Boltzmann simulations have also demonstrated that the surface-tension coefficient σ is a constant independent of the radius of a drop.

Over the past three years, several Los Alamos scientists and several scientists from Mobil Oil Company have developed a collaboration, applying the two-phase model to study flows through porous media. The results of simulations in two and three dimensions are shown in the companion article. The goal of the collaboration is to develop a greater understanding of the fundamental physics related to enhanced oil recovery, and to predict relative permeabilities and other bulk properties of porous media from basic properties of the fluid-fluid and fluid-rock interactions. So far, lattice-Boltzmann simulations look promising: Initial results compare well with experimental measurements of flow patterns and relative permeabilities.

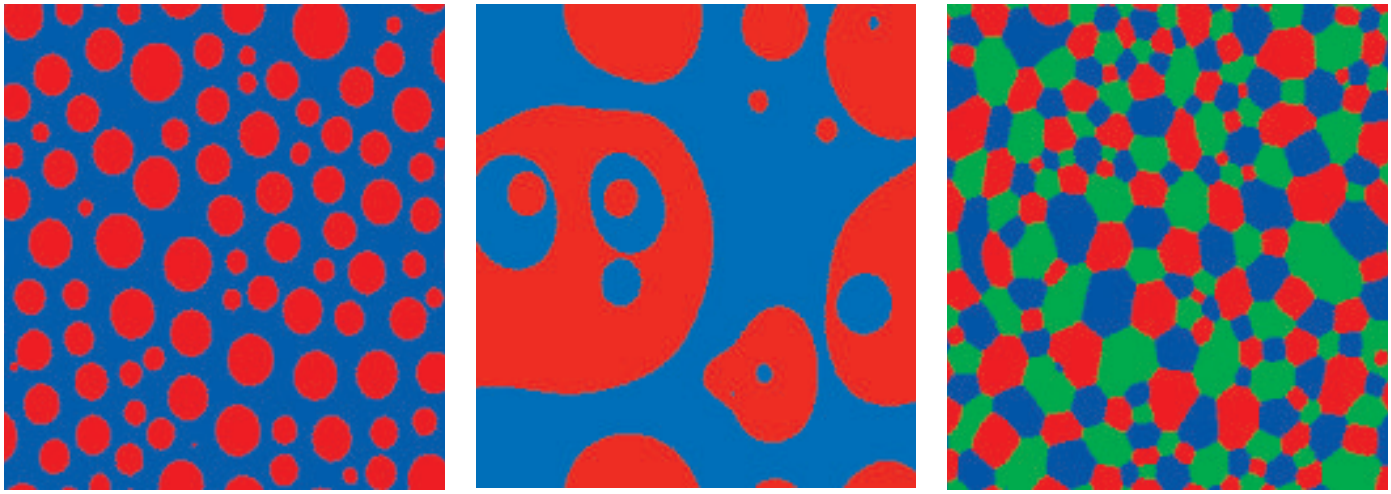


Figure 8. Lattice-Boltzmann Simulations of Phase Separation

Each of the three figures is a snapshot of a lattice-Boltzmann simulation after 6000 timesteps, starting from an initial random distribution of the phases present. (a) The red and blue densities are 0.4 and 0.6, respectively. Since the density of the red fluid is lower than that of the blue, red drops form in a blue background. At each site the lattice-Boltzmann simulation produces, in essence, an ensemble average of lattice-gas simulations, so the boundaries between the red and blue fluids are much smoother in this simulation than in the corresponding lattice-gas simulation shown in Figure 4. (b) The densities of the red and blue fluids are 0.5 and 0.5. Phase separation again takes place readily but produces a different pattern than in (a) because the densities of the two phases are equal. (c) The model for immiscible fluids can be applied to any number of phases. Here there are three phases, red, blue, and green, and each has a density equal to 0.33. Again the three phases separate from an initial random distribution.

Applications and Extensions

Lattice multiphase models have been used for investigating the details of interface dynamics, including the well-known phenomena Rayleigh-Taylor instability, Saffman-Taylor instability, and domain growth in the separation of two immiscible fluids (see Figure 8). The two-phase lattice-Boltzmann model has been extended to three and four phases to study critical and off-critical quenches and phase transitions.

Features of interest in biological problems have also been added to lattice-Boltzmann models. For example, the addition of a surfactant fluid to two-phase flows is being used to study the formation of lipid bilayers. If one end of the surfactant prefers the red fluid and the other end of the surfactant prefers the blue fluid, the fluids are forced to have a much more extensive interface. This approach is being used for studying the self-assembly of biological membranes, surfactant effects in two- and three-dimensional multiphase models, the formation of membranes, and self-assembly of amphiphilic structures at aqueous organic interfaces.

Simple reaction-diffusion systems are also being modeled with lattice-Boltzmann methods. Recent work has shown that these simple systems can exhibit extremely complicated and unexpected behavior. For example, solutions have been found that behave like biological cells; that is, concentrations of chemical densities within well-defined regions of the solution divide as cells divide.

The lattice-Boltzmann method, like any new method, is going through an exploratory stage to determine its limitations and optimal areas of application. Recently, stability analyses have been completed, and the conditions under which the method becomes unstable (as do all finite-difference schemes) have been determined. When the allowed number of speeds is increased from three to many, a thermohydrodynamic version of the lattice-Boltzmann method emerges. Such a model has been developed and tested by several scientists. The current lattice models for reacting systems are based on simple isothermal models, but they can easily be extended to include temperature effects and to model phase transitions in which the reaction rate depends on local temperature.

Clearly, the lattice-Boltzmann method is still in the developmental stages. Because it is relatively straightforward to introduce new physics into the model, we expect it will be applied to many additional physical phenomena. ■

Acknowledgements

Members of the Lattice-Boltzmann Research Effort: Francis Alexander, Mario Ancona, Daryl Grunau, Brosl Hasslacher, Shuling Hou, Nathan Kreisberg, Turab Lookman, Lishi Luo, Daniel Martinez, Guy R. McNamara, Balu Nadiga, Silvina Ponce-Dawson, Xiaowen Shan, James Sterling, and Qisu Zou.

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Seated at the monitor, Shiyi Chen; standing, left to right, Gary D. Doolen, Kenneth G. Eggert, and Wendy E. Soll. [Soll is a co-author of "Toward Improved Prediction of Reservoir Flow Performance."]

Shiyi Chen first joined the Laboratory as a postdoctoral fellow in 1987; he was an Oppenheimer Fellow from 1990 to 1992. In 1992 he became a staff member in the Complex Systems Group of the Theoretical Division. His research interests include lattice-gas automata and lattice-Boltzmann computational methods, the statistical theory of fluid turbulence, and two-phase and compressible fluid flows. A native of the People's Republic of China, Chen earned his B.S. in 1981 from Zhejing University and his M.S. and Ph.D. from Beijing University in 1984 and 1987.

Gary D. Doolen joined the Laboratory's Applied Theoretical Physics Group in 1975. His research interests include nuclear physics, plasma physics, magnetohydrodynamics, neural networks, and nonlinear mathematics. Doolen was with the Center for Nonlinear Studies from 1988 through 1993. He is now the leader of the Complex Systems Group. He received his B.S. in engineering science in 1961 and his M.S. and Ph.D. in physics in 1964 and 1967 from Purdue University.

Kenneth G. Eggert joined the Laboratory's Geoanalysis Group as a section leader in 1987 and became group leader in 1992. His research interests include use of simulation in the management of surface and subsurface hydrologic systems, physics of multiphase flow, and parallel computation in the earth sciences. From 1984 to 1987 he was a physicist in the Earth Sciences Department at Lawrence Livermore Laboratory where he participated in the Yucca Mountain Project. Eggert received his B.S. in aerospace engineering from Purdue University in 1969 and his M.S. and Ph.D. in civil engineering from Colorado State University at Fort Collins in 1976 and 1980. Eggert is a member of the Society of Petroleum Engineers and the American Geophysical Union.

Equations of the Lattice-Boltzmann Method

The Boltzmann equation for any lattice model is an equation for the time evolution of $f_i(\mathbf{x},t)$, the single-particle distribution at lattice site $\mathbf{x}$:

$$f_i(\mathbf{x} + \mathbf{e}_i,\, t + \Delta t) = f_i(\mathbf{x},t) + \Omega_i(f(\mathbf{x},t)),$$

where $\Omega_i = \Omega_i(f(\mathbf{x},t))$ is the local collision operator at that site, $i = 0,1,\ldots,14$, and Δt is assigned a value of unity. Since the usual aim of lattice methods is to model macroscopic dynamics, the "exact" collision operator is unnecessarily complex and therefore numerically inefficient. Two groups (see Chen *et al*. and Qian *et al.* in the Further Reading) nearly simultaneously suggested that the collision operator be approximated by a single-time-relaxation process in which relaxation to some appropriately chosen equilibrium distribution occurs at some constant rate. In particular the collision term, $\Omega(f)$, is replaced by the single-time-relaxation approximation,

$$\Omega_i(f(\mathbf{x},t)) = -\frac{f_i(\mathbf{x},t) - f_i^{\mathrm{eq}}(\mathbf{x},t)}{\tau}.$$

The appropriately chosen equilibrium distribution, denoted by f^{eq}, depends on the local fluid variables, and $1/\tau$ is the rate of approach to this equilibrium. The relations $\sum_i \Omega_i = 0$ and $\sum_i \mathbf{e}_i \Omega_i = 0$ must be true to conserve mass and momentum, respectively. In order for the fluid to have Galilean-invariant convection and a pressure that does not depend on velocity, an appropriate equilibrium distribution, f_i^{eq}, must be assumed. For a two-dimensional hexagonal lattice, the formula is:

$$f_i^{\mathrm{eq}} = \frac{\rho(1-\alpha)}{6} + \frac{\rho}{3}\mathbf{e}_i\cdot\mathbf{v} + \frac{2\rho}{3}(\mathbf{e}_i\cdot\mathbf{v})^2 - \frac{\rho}{6}\mathbf{v}^2$$

and

$$f_0^{\mathrm{eq}} = \alpha\rho - \rho\mathbf{v}^2.$$

(The corresponding formulas for the cubic lattice appear in the article by Alexander, Chen, and Grunau listed in the Further Reading.) In these equations the density $\rho(\mathbf{x},t) = mn(\mathbf{x},t)$ (where m is the mass of each particle), the number density $n(\mathbf{x},t) = \sum_i f_i(\mathbf{x},t)$, and α is a free parameter related to the sound speed as shown below. For the lattice-Boltzmann method, the particle distribution does not have an upper bound. The only requirement is that $f_i \geq 0$.

To derive the macroscopic equations obeyed by this model, one performs a Taylor expansion in time and space and takes the long-wavelength and low-frequency limit of the lattice-Boltzmann equation for the single-particle distribution. The result is a continuum form of the Boltzmann equation correct to second order in the lattice spacing and the timestep. A scaling expansion argument, the assumption of single-time relaxation, and the neglect of higher-order terms lead to the following final form of the macroscopic equations obeyed by the simulated system

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho v_\beta)}{\partial x_\beta} = 0,$$ the equation of mass continuity;

$$\frac{\rho \partial v_\alpha}{\partial t} + \rho v_\beta \frac{\partial v_\alpha}{\partial x_\beta} = -\frac{\partial p}{\partial x_\alpha} + \frac{\partial}{\partial x_\beta}\left[\frac{\lambda}{\rho}\left(\frac{\partial \rho v_\gamma}{\partial x_\gamma}\delta_{\alpha\beta} + v_\alpha \frac{\partial \rho}{\partial x_\beta} + v_\beta \frac{\partial \rho}{\partial x_\alpha}\right)\right] + \frac{\partial}{\partial x_\beta}\left[\mu\left(\frac{\partial v_\beta}{\partial x_\alpha} + \frac{\partial v_\alpha}{\partial x_\beta}\right)\right],$$

the equation of momentum conservation; and

$$p = \frac{1-\xi}{2}\rho.$$

the equation of state.

In the above equations, v_β is the component of the velocity in the β-direction; p is the pressure; and the sound speed, c_s, is $\sqrt{(1-\xi)/2}$, where ξ is a free parameter. The shear viscosity, μ, and the bulk viscosity, λ, are given by

$$\mu = \frac{2\tau - 1}{8}\rho$$

and

$$\lambda = \frac{(\tau - 1/2)(2\xi - 1)}{4}\rho.$$

The above equations converge to the exact incompressible Navier-Stokes equations only when the derivatives of the number density in the second viscosity term on the right-hand side of the equation are small. Since the gradients of the density are O(v^2), the unphysical terms in the momentum-conservation equation are correct to order (v^3). Thus, although the physics of the lattice-Boltzmann method contains compressibility effects, one may come arbitrarily close to solving the incompressible Navier-Stokes equations by reducing the Mach number (through the choice of α) and thereby reducing the simulated flow to very low speed. (Nevertheless the compressibility effects in the lattice-Boltzmann approach are physical and the method can also be used to simulate compressible fluids.)

Traditional methods for solving incompressible flows, such as finite-difference or finite-element, require solution of a Poisson equation for the pressure term, which is induced by the mass-continuity equation and the momentum-conservation equation. In the lattice-Boltzmann approach, this time-consuming step is avoided because the incompressibility requirement has been relaxed and the effects of pressure changes are controlled by an equation of state rather than a Poisson equation. It can be argued that the conventional methods most closely related to the lattice-Boltzmann method are the pseudocompressible algorithms for solving incompressible fluid flows. □