Microscopic and Macroscopic
Cellular-Automaton Simulations
of Fluid Flow and Wave Propagation
in Rocks

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Saskatoon

By
Jianwu Jiao

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Microscopic and Macroscopic Cellular-Automaton Simulations of Fluid Flow and Wave Propagation in Rocks

Lattice-Gas Automata (LGA) and their extension, Lattice-Boltzmann (LB) methods have emerged in recent years as alternatives for modeling. This dissertation is intended to demonstrate applications of this relatively new approach to simulations of fluid flow and wave propagation in porous media. In supporting this objective, the basis for several efficient and accurate naturally-parallel computational schemes are introduced for reservoir simulation and seismic modeling.

After laying the theoretical basis of LGA and LB methods in the context of incompressible hydrodynamics, reservoir simulation algorithms are derived, based on the LB version of the Bhatnagar, Gross, and Krook (BGK) collision model, for single-phase Darcy flow, miscible displacement processes, and immiscible displacement processes, respectively. The single-phase model allows simulation of a wide range of permeabilities for both compressible and incompressible fluid flows. The simulation results for several, one-dimensional (1D) or two-dimensional (2D) steady or unsteady state flows are shown to be in good agreement with their corresponding analytical solutions. By comparing the analytic solutions for the 1-D convection-diffusion equation with results of the miscible model, it is obvious that the latter is capable of resolving sharp displacement fronts in convection-dominated flows. The miscible model is also shown to be convergent and insensitive to grid orientations and to be capable of handling instabilities due to perturbation in 2-D displacements with unfavorable mobility ratios. Computations of unstable displacements illustrate fingering evolutions very similar to those determined experimentally. The immiscible model is verified with the Buckley-Leverett problem and repeated five-spot pattern by analytical and finite difference methods. Significant reductions in the diffusion of sharp fronts and in sensitivity to grid orientation result as compared to low-order finite difference schemes.

The LB approach is developed for simulations of seismic wave propagation in inhomogeneous media. Acoustic waves can be simulated using the fluid models when perturbations of the idealized fluid are small. It is demonstrated theoretically and numerically that the macroscopic behavior of the LB acoustic model corresponds to that of a linear acoustic equation. Experiments performed on serial computers indicated that the LB scheme has a better relative performance than the second-order central-differencing scheme though the former is typically considered to be a second-order method. While it is natural to extend the fluid-based LB model to the simulation of acoustic waves, the LB model for elastic waves is motivated by the similarity between the Navier-Stokes equation and the elastic wave equation. The resulting algorithm permits an accurate and robust implementation that involves both free surface and absorbing boundary conditions. Comparisons between numerical results obtained from the LB model and an analytical approach based on the Cagniard technique for Lamb’s problem verify the approach.

The capabilities of lattice methods for the microscopic simulation and evaluation of various rock parameters, particularly, LGA calculations of permeability and LB determination of seismic wave attenuation, are demonstrated. Models confirm Darcy’s law for Poiseuille flow, a given complicated boundary flow and fractal geometry flow. The LGA hydrodynamic model is also applied to the problem of simulating binary fluids and demonstrating the effects of surface tension. Finally, the LB acoustic model is used to investigate seismic wave propagation in media filled with fractal cracks or inclusions.
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Abstract

Lattice-Gas-Automata (LGA) methods and their extension, Lattice-Boltzmann (LB) methods, have emerged in recent years as alternatives for modeling fluid dynamics and other systems described by partial differential equations. These schemes do not attempt to directly solve the equations, but rather to create a dynamics of fictitious particles in a lattice, whose macroscopic behavior corresponds to the Navier-Stokes equations or the equations of interest.

In a field largely dominated by well-established algorithms based on finite-difference, finite-element and spectral methods, these lattice schemes have survived, thus far, because of their simplicity and parallel nature. However, only in the event that practitioners of LGA and LB methods test their validity with rigor, will they endure. This dissertation is intended to demonstrate applications of this relatively new approach to simulations of fluid flow and wave propagation in porous media. In supporting this objective, the basis for several efficient and accurate naturally-parallel computational schemes are introduced for reservoir simulation and seismic modelling.

After laying the theoretical basis of LGA and LB methods in the context of incompressible hydrodynamics, reservoir simulation algorithms are derived, based on the LB version of the Bhatnagar, Gross, and Krook (BGK) collision model, for single-phase Darcy flow, miscible displacement processes, and immiscible displacement processes, respectively. The single-phase model allows simulation of a wide range of permeabilities for both compressible and incompressible fluid flows. The simulation results for several, one-dimensional (1D) or two-dimensional (2D) steady or unsteady state flows are shown to be in good agreement with their corresponding analytical solutions. By comparing the analytic solutions for the 1-D convection-diffusion equation with results of the miscible model, it is obvious that the latter is capable of resolving sharp displacement fronts in convection-dominated flows. The miscible model is also shown
to be convergent and insensitive to grid orientations and to be capable of handling instabilities due to perturbation in 2-D displacements with unfavorable mobility ratios. Computations of unstable displacements illustrate fingering evolutions very similar to those determined experimentally. The immiscible model is verified with the Buckley-Leverett problem and repeated five-spot pattern by analytical and finite difference methods. Significant reductions in the diffusion of sharp fronts and in sensitivity to grid orientation result as compared to low-order finite difference schemes.

The LB approach is developed for simulations of seismic wave propagation in inhomogeneous media. Acoustic waves can be simulated using the fluid models when perturbations of the idealized fluid are small. It is demonstrated theoretically and numerically that the macroscopic behavior of the LB acoustic model corresponds to that of a linear acoustic equation. Experiments performed on serial computers indicated that the LB scheme has a better relative performance than the second-order central-differencing scheme though the former is typically considered to be a second-order method. While it is natural to extend the fluid-based LB model to the simulation of acoustic waves, the LB model for elastic waves is motivated by the similarity between the Navier-Stokes equation and the elastic wave equation. The resulting algorithm permits an accurate and robust implementation that involves both free surface and absorbing boundary conditions. Comparisons between numerical results obtained from the LB model and an analytical approach based on the Cagniard technique for Lamb’s problem verify the approach.

The capabilities of lattice methods for the microscopic simulation and evaluation of various rock parameters, particularly, LGA calculations of permeability and LB determination of seismic wave attenuation, are demonstrated. Models confirm Darcy’s law for Poiseuille flow, a given complicated boundary flow and fractal geometry flow. The LGA hydrodynamic model is also applied to the problem of simulating binary fluids and demonstrating the effects of surface tension. Finally, the LB acoustic model is used to investigate seismic wave propagation in media filled with fractal cracks or inclusions.
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Chapter 1

Lattice–Gas and Lattice–Boltzmann Methods

1.1 Introduction

The analysis of fluid flow and wave propagation in rocks has a long history in connection with the production of oil from underground reservoirs. However, it is only in the past fifteen years that this analysis has been extensively extended to include detailed structural properties of the media. These studies are quite diverse in the physical phenomena that they consider. Conventionally, we could classify the models for fluid flow and wave propagation in reservoir rocks as continuum models and discrete models. Continuum models represent the classical engineering approach to describing materials of complex and irregular geometry, characterized by several length scales. The physical laws that govern fluid transport and wave propagation at the microscopic level are well understood, with the exception of ultramicroporous structures. Leaving aside that case, one could in principle write down differential equations for motion, energy, and mass and the associated initial and boundary conditions at the fluid–solid interface. However, as the interface in typical rocks is very irregular, practical and economical techniques are not available for solving boundary-value problems—even in the unlikely event that one knows the detailed morphology of the medium. Determination of the precise solid–fluid boundary in any rock is, and will probably remain, a very difficult (if not impossible) task; the boundary (even if known) within which
one would have to solve the equations of change would be so tortuous as to render
the problem mathematically intractable. Moreover, even if the solution of the problem
could be obtained in such great detail, it would contain much more information than
would be useful in any practical sense. Thus it becomes essential to adopt a macro-
scopic description at a length scale much larger than the dimension of individual pores
or fractures.

1.1.1 Continuum and discrete models

Macroscopic properties such as effective transport coefficients and elastic constants
are defined as averages of the corresponding microscopic quantities (see, for example,
Slattery, 1967, 1969; Whitaker, 1967; Gassmann, 1951; Biot, 1956; de la Cruz and
Spanos, 1985). The averages must be taken over a representative volume that is small
enough compared to the volume of the system, but large enough for the equation of
change to hold when applied to that volume. At every point in the medium one uses
the smallest such volume and, thereby, generates macroscopic field variables obeying
equations such as Darcy’s law of flow. The reasons for choosing the smallest suit-
able volume for averaging are to allow superpore variations of the porous medium
and to generate a theory capable of treating the usual macroscopic variations of ef-
fective properties. In any case, with empirical, approximate, or exact formulae for
the transport coefficients, elastic constants, and other effective properties, the results
of a given phenomenon in a porous medium can be analyzed with the macroscopic
partial differential equations based on the classical description of the system as a
continuum. We shall therefore refer to various models associated with this classical
description as continuum models. These models have been widely applied to simula-
tions of reservoir fluid flow and seismic wave propagation because of their convenience
and familiarity to engineers and geophysicists. Many numerical techniques, includ-
ing the finite-difference method, finite-element method, boundary-element method,
and spectral method, have been developed to solve these differential equations with
complex geological structures arising from reservoir engineering. However, they do
have some limitations, one of which was noted above in the discussion concerning
scales and averaging. They are also not well suited for describing those phenomena in
rocks in which the connectivity of the pore space or a fluid phase plays a major role,
for example, in dispersion and capillarity. Such models also break down if there are long-range correlations in the system.

The second class of models, the discrete models, are free of these limitations. These models have been advanced to describe phenomena at the microscopic level and have been extended in the last few years to describe various phenomena at the macroscopic level. Their main shortcoming, from a practical point of view, is the large computational effort required for a realistic discrete treatment of the system. They are particularly useful when the effect of the pore-space interconnectivity or long-range correlations is strong. Most of the discrete models are based on a network representation of the rock. The original idea of network representation of a pore space is rather old, but it was only in the early '80s that systematic and rigorous procedures were developed (Lin and Cohen. 1982) to map, in principle, any disordered rock onto an equivalent random network of bonds and sites. Once this mapping is complete, one can study a given phenomenon in porous media in great detail. However, only in the past fifteen years have ideas from the statistical physics of disordered media been applied to fluid flow and wave propagation in porous rocks. These concepts include percolation theory (Stauffer and Aharony, 1992), the natural language for describing connectivity effects, diffusion limited growth processes (Meakin, 1991), which describe fundamentally nonequilibrium growth processes, fractal concepts (Mandelbrot, 1982; Bunde and Havlin, 1991), which are the main tool for describing the self-similarity and self-affinity of the morphology of a system and the effect of long-range correlations, and universal scaling laws, which describe how and under what conditions the effective macroscopic properties of a system may be independent of its microscopic details.

1.1.2 Reservoir simulation and seismic modeling

Simulation of multiphase, multicomponent flows and seismic wave propagation in natural porous media are often called reservoir simulation and seismic modeling in the petroleum industry. The reservoir simulations that are normally used in the petroleum industry are usually one of two types. The first type is the so-called black oil simulator, in which it is assumed that the fluids (usually oil, gas, and water) are homogeneous. It is also assumed that gas can dissolve in the oil, or vice versa, in any given proportion. This avoids the problem of computing the detailed phase diagrams of the
system, which requires accurate equations of state. The second type of simulator is more complex. Usually called a compositional simulator, it represents the oil as a mixture of several hydrocarbons and performs detailed phase equilibria calculations in order to determine the distribution of components between the liquid and vapor phases in the reservoir. Prior to the introduction of supercomputers, seismic modeling was essentially confined to 1-D and 2-D ray tracing. Ray tracing modeling is still a widely used seismic modeling technique. However, in instances where there is complex geology or complex wave phenomena, geophysicists do turn to acoustic or elastic wave-equation modeling. Initially, with limited computing power, wave-equation modeling was primarily used for fundamental research studies. Now, however, wave-equation modeling is used more often to test seismic interpretation, to plan data acquisition, and to calibrate the effectiveness of seismic processing schemes (and other modeling programs). We also use forward modeling schemes in inversion, but a typical model-driven inversion program requires ten or more forward simulations, which requires even greater computational power.

In most reservoir simulations and seismic modeling the preferred numerical method is a finite-difference approximation to the transport and wave equations. The reservoir is divided into blocks. A five-point (in two dimensions) or seven-point (in three dimensions) finite-difference approximation is most commonly used. This has both advantages and disadvantages. The main advantage of using a finite-difference method is that it is straightforward to set up the discretized transport and wave equations that are to be solved. The main disadvantage results when large blocks are used which may lead to numerical dispersion which is often used to mimic physical dispersion. However, numerical errors cannot model physical processes. While this can be advantageous, if physical dispersion is actually present, it can be a disadvantage, in the sense of producing solutions that do not actually approximate the true situation.

In any event, once the equations are set up, they are usually solved by iterative methods. Nonlinear transport equations are also linearized and solved using the Newton–Raphson method. Direct methods such as Gaussian elimination are rarely used (although, in principle, they are much more accurate than iterative methods), simply because the number of equations is so large that no computer memory can fit the enormous matrix of the coefficients. even though these matrices are usually sparse
and banded. Solving these equations by iterative methods means that there has to be a 
tradeoff between the desired accuracy of the solution and the available computer time 
in order to achieve that accuracy. Another problem with finite-difference methods is 
that they are not suitable for systems that have complex boundaries, unless the dis-
cretization is very refined. But a very refined discretization also implies a much larger 
number of equations to be solved. Various finite-element methods are better suited 
for such computations and can overcome the worst numerical dispersion problems, 
but the matrix of coefficients in finite-element methods is usually full and dense, not 
sparse and banded as in finite-difference methods.

For these reasons, devising efficient numerical methods for solving the transport 
and wave equations has always been an active area of research. Detailed review 
will be presented in Section 2.1 and Section 3.1 on numerical methods for reservoir 
simulation and wave equation modeling, respectively. However, we will discuss a 
new method of simulating fluid flow and wave propagation in porous media based 
on cellular automata (CA), or lattice gases (LG) and their extension to the lattice-
Boltzmann (LB) methods, which we believe can dramatically change the way people 
think about simulation of fluid flow and wave propagation in porous media as well 
as reservoir simulation and seismic modeling. After introducing the CA methods in 
Subsection 1.1.3. the following two sections are devoted to reviews of the basic ideas 
about lattice-gas and lattice-Boltzmann methods and the recent advances in these 
subjects.

### 1.1.3 Cellular automaton methods

Cellular automata (for reviews see Wolfram, 1986; Doolen, 1989, 1991; Boon, 1992) 
are large lattices in which each site can be in one of several discrete states. The 
state of each site at the next time step is determined completely by the present state 
of the neighboring sites. Thus both time and space are discrete, and connections 
are between neighbors only, which are ideal conditions for high-speed simulations 
on vector or parallel computers. The CA approximation (lattice-gas model) of the 
Navier-Stokes equation in two dimensions is based on particles of unit mass either 
resting on the site of a lattice or moving with unit velocity on one of the six bonds 
emanating from each lattice site. Frisch et al. (1986), using a model developed by
Hardy et al. (1973, 1976), showed that in order that the discrete equations reduce to the usual Navier–Stokes equations, two-dimensional simulations have to be done on a hexagonal lattice.

Why should we expect that the average behavior of discrete particles on a lattice will be like that of a fluid? The answer was perhaps put most eloquently by Feynman as quoted by Hills (1989): “We have noticed in nature that the behavior of a fluid depends very little on the nature of the individual particles in that fluid. For example, the flow of sand is very similar to the flow of water or the flow of a pile of ball bearings. We have therefore taken advantage of this fact to invent a type of imaginary particle that is especially simple for us to simulate. This particle is a perfect ball bearing that can move at a single speed in one of six directions. The flow of these particles on a large enough scale is very similar to the flow of natural fluids.”

Since computations involving cellular automata are performed using fixed-point arithmetic (and, therefore, have no roundoff error), it is interesting and, perhaps, slightly ironic that a new floating-point method has arisen from lattice–gas theory (McNamara and Zanetti, 1988; Higuera and Jimenez, 1989; Qian et al., 1992). The lattice–Boltzmann method first arose as an attempt to simulate the Boltzmann equation for a lattice–gas rather than the lattice–gas itself. The same sort of lattice is used, but instead of using bits to represent discrete particles at each site, floating-point numbers are used to represent the mean occupation number of particles on each link of the lattice. Like the bits of the lattice–gas, these floating-point numbers move to neighboring sites at each timestep; there they “collide” by forming algebraic (rather than logical) combinations that conserve the relevant quantities. Shortly after lattice–Boltzmann methods were introduced, it was realized that they did not have to be based on underlying lattice–gas models, and the method was generalized in some important ways.

CA methods, including the lattice–gas method and the lattice–Boltzmann method, are now becoming powerful alternatives to traditional numerical schemes for solving partial differential equations and modeling physical systems, particularly for simulating fluid flows whose dynamics are described by the Navier–Stokes equation. In finite-difference and finite-element methods, the given macroscopic equation is solved by some specific numerical discretization while in full molecular dynamics descrip-
tions, each individual particle is closely and accurately followed. Unlike these traditional numerical schemes, the idea behind lattice-gas and lattice-Boltzmann methods is to construct a simplified molecular dynamics that incorporates many of the essential characteristics of the real microscopic processes so that the macroscopic averaged properties obey the desired macroscopic equations. The CA methods can be described as a mesoscopic model which occupies a position between full molecular dynamics and macroscopic descriptions by means of partial differential equations.

Even though CA models originate from a particle picture, they are mainly focused on averaged macroscopic behavior. In most cases CA methods are developed as numerical schemes rather than microscopic models for understanding fundamental physics. However, the utilization of the particle description or the kinetic equation provides some of the advantages of molecular dynamics, including clear physical pictures, easy implementation of boundaries and fully parallel algorithms.

The development of a CA model includes the following three steps: (i) the construction of the model, (including the design of a particle collision operator and the choice of conservation rules); (ii) the derivation of the macroscopic dynamics: for most cases, this step involves a Chapman-Enskog expansion or a multiscaling analysis\(^1\); (iii) the numerical validation of the theory and application of the model to real situations. For a given macroscopic equation, the design of the corresponding microscopic CA method is an inverse problem. There are no general principles to guarantee that one can find such a lattice-gas model. Nevertheless, many CA models already exist for solving partial differential equations, including the Navier-Stokes equations (Frisch et al., 1986, 1987; Clavin et al., 1988; Kadanoff et al., 1989; Benzi et al., 1993; Chen S. et al., 1992). Burgers’ equation (Boghosian and Levermore, 1987; Cheng et al., 1991), the Poisson equation (Chen H. et al., 1990), the wave equation (Rothman, 1987; Chen H. et al., 1988a; Huang et al., 1988; Mora, 1992), the diffusion equation (Ladd et al., 1988; Binder, 1989; Binder and d’Humieres, 1989; Qian et al., 1993); and for modeling physical phenomena, including flow through porous media (Balasubramaniam et al., 1987; Rothman, 1988; Succi et al., 1989; Chen S. et al., 1991a:

\(^1\)The Chapman-Enskog expansion (1952) is a multiple-time formulism of multiscaling perturbation analysis where both function and its time derivatives are power series of a single parameter. Sydney Chapman (1888–1970) was a well-known geophysicist.

It is natural to use CA methods for simulating compressible fluids because of the intrinsic compressibility in the particle representation. Most models developed so far, however, are mainly focused on the incompressible limit of the CA methods. Recent numerical simulations (Reider and Sterling, 1993) have demonstrated that the solution of the CA methods converges to the solution of the Navier–Stokes equation for flow velocities much smaller than the sound speed.

Most two-dimensional lattice–gas models have been based on the hexagonal lattice. Three-dimensional lattice–gas models are based on the face-centred-hypercubic lattice (d'Humieres et al., 1986) dictated by the isotropy requirements for the stress tensor and convection term in the Navier–Stokes equation. Lattice–Boltzmann methods can be adapted to many different lattices, such as the 9-directional square lattice (Qian et al., 1992; Martinez et al., 1993) in two dimensions and the body-centered cubic lattice in three dimensions (Chen, S. et al., 1992; Qian et al., 1992). In order to focus on the fundamental principles of the CA methods, we will only discuss dynamics based on the hexagonal lattice in this chapter.
1.2 Lattice–Gas Method

Lattice–gas methods for hydrodynamic systems were originally proposed by Hardy, de Pazzis and Pomeau (HPP) (1976) on a square lattice in two dimensions for understanding transport properties in hydrodynamics. Serious problems in the square lattice include spurious momentum conservation and anisotropy of the stress tensor. The important contribution made by Frisch, Hasslacher and Pomeau (FHP) (1986) was to show that a hexagonal lattice–gas model has an isotropic stress tensor and almost eliminates the spuriously conserved quantities.

Lattice–gas methods locally conserve total mass, momentum and energy exactly, with no round–off error, therefore these algorithms are unconditionally stable. Moreover, lattice–gas methods can easily handle very complicated geometry and boundary conditions. For example, the nonslip condition can be implemented by particle velocity reversal at the boundaries.

There are many reasons for studying lattice–gases, both practical and theoretical. Some commonly cited reasons are oriented towards computer science and issues related to massively parallel processing. There are also appealing reasons related to modeling physical systems with complex boundary conditions. The lattice–gas attributes include: 1) bit efficiency; 2) inherent simplicity; 3) logic density; and 4) exact computability.

Firstly, lattice–gas automata allow for high bit efficiency. A single digital bit is used to represent a particle. Unlike floating–point calculations where there exist uncontrolled round–off errors in the least significant bits, in lattice–gases all bits have equal weight, or to quote Frisch, there is “bit democracy.” Consequently, the efficiency with which bits are used should be higher for lattice–gases.

Secondly, lattice–gas automata possess an inherent simplicity. Just as simple models in statistical mechanics, such as the Ising model, shed light on equilibrium critical phenomena, lattice–gas models shed light on dynamical phenomena. Moreover, their inherent simplicity gives them pedagogical value since many properties of macroscopic systems can be understood through analytical expressions given very simple local rules. For example, lattice–gases are a simple way to understand details of fluid systems such as the dependence of the shear viscosity on particle collision rates.
Computational fluid dynamics codes are complicated and intricate in their approximations. Lattice-gases are perhaps the simplest expression of Navier-Stokes flows and are easily implemented.

Thirdly, the combination of bit efficiency with the simplicity and locality of some lattice-gas rules allows—in principle—nearly ideal logic density. At the highest logic density that is physically possible, there is the interesting prospect of lattice-gas architectures built out of “quantum hardware.” There is the expectation that in the future, computation will be achieved on quantum computers (Margolus, 1990). As the fundamental computational element’s size reduces to nano-scale ranges its behavior is governed by quantum mechanics. Quantum mechanics requires unitary, and hence invertible, time evolution—the microscopic reversibility of the lattice-gas dynamics is important here. Even before quantum mechanics becomes a constraint, the reversibility of lattice-gas dynamics may become a significant benefit, since at very high logic densities the dissipation of heat caused by irreversible computations will become an issue (Bennett, 1982).

Fourthly, lattice-gas automata are exactly computable. Richard Feynman (1982) considered on a discrete spacetime lattice “the possibility that there is to be an *exact* simulation, that the computer will do *exactly* the same as nature”, and that using computers in an exactly computable way may lead to new possibilities in our understanding of physics. Although lattice-gases cannot model quantum systems, they do model classical systems while keeping mass, momentum, and energy exactly conserved. Exact modeling is valuable, for example, in cases where multiparticle correlations are essential to the system’s behavior. Lattice-gas simulations can verify theoretical predictions beyond the Boltzmann mean-field approximation of uncorrelated collisions: the phenomenon of long-time tails in the velocity autocorrelation function has recently been observed in lattice-gases (Kirkpatrick and Ernst, 1991; Brito and Ernst, 1992).

However, there are two main limitations for lattice-gas models in the simulation of fluid flows. First, the Reynolds numbers and Mach numbers can not be too large. On existing large computers, Reynolds numbers up to 10,000 can be modeled in two dimensions and up to 1000 in three dimensions. The incompressible Navier-Stokes equation is derivable only in the low Mach number limit (Majda, 1984). This restriction can be relaxed if one uses multiple discrete velocity models.
Second, local quantities in lattice-gas models are usually noisy, requiring spatial and time averaging in order to study the macroscopic dynamics. This requires large computer memory or long computational time. On the other hand, fluctuations are important for studying several physical details, such as noise-driven pattern formation. The lattice-gas method is particularly suitable for these purposes. Lattice-Boltzmann methods, in which real numbers replace the bits in a lattice-gas model, greatly reduce these fluctuations.

Furthermore, there are two unsolved problems when one uses the lattice-gas method for simulating the Navier-Stokes fluids: the non-Galilean invariance of convection and the velocity dependence of the equation of state (Frisch et al., 1987). Both problems are effects of the restriction to a finite number of velocities and the Fermi-Dirac statistics employed to minimize memory requirements.

The basic two-dimensional FHP lattice-gas model consists of identical particles moving on a hexagonal lattice. The lattice spacing, $c$, is unity and all particles have the same mass, momentum magnitude and kinetic energy, except for rest particles which are often included in order to increase the Reynolds number range. There are six nonzero momentum states associated with the directions to the nearest neighbors. An exclusion principle is usually imposed which requires that no more than one particle at a given site can have the same momentum. This exclusion rule is included in order to minimize memory requirements and to allow bit operators. Let $N_i(x,t)$ $(i = 0, 1, \ldots, 6)$ be the particle occupation in state $i$ at site $x$ and time $t$, then $N_i = 1$ or $0$ represents a particle existence in the $i$ state. Similar to classical molecular dynamics, there are two microscopic updating processes at each discrete time step: streaming (particle moving) and particle collision. In the streaming process, particles move to the nearest neighbor sites along their momentum directions. In the collision process, particles at each site are scattered in such a way that the total particle number $(\sum_{i=0}^{6} N_i)$ and the total momentum $(\sum_{i=0}^{6} e_i N_i)$ are conserved at each site, where $e_i (i = 1, \ldots, 6)$ is the unit vector pointing to the nearest neighbors and $e_0 = 0$. The kinetic equation for the particle state occupation can be written in a simple form,

$$N_i(x + e_i, t + 1) = N_i(x, t) + \Omega_i,$$  \hspace{2cm} (1.1)

where $\Omega_i$ is the collision operator, which includes the creation or annihilation of a
particle in momentum state $e_i$ and only depends on the information at the site $x$ at time $t$. The collision operation has the form (Frisch et al., 1987):

$$\Omega_i = \sum_{s,s'} (s' - s) \xi(s \rightarrow s') \prod_j N_j^{s'} (1 - N_j^{s'})^{1-s_j}.$$  

(1.2)

In the above equation, $s = (s_0, s_1, s_2, \ldots, s_8)$ and $s'$ represent the local states before and after collision and $\xi(s \rightarrow s')$ is a Boolean matrix with expectation, $\langle \xi(s \rightarrow s') \rangle$, equal to the transition probability $P(s \rightarrow s')$ from state $s$ to $s'$. The conservation of mass and momentum requires the collision operator to satisfy $\sum_{i=0}^{8} \Omega_i = 0$ and $\sum_{i=0}^{8} e_i \Omega_i = 0$. To allow the system to approach a local equilibrium, the microscopic collision transition probability $P$ usually satisfies the semi-detailed balance condition: $\sum_s P(s \rightarrow s') = 1$.

Some simple collision processes are illustrated in Figure 1.1. If we let $f_i = \langle N_i \rangle$ be the ensemble-averaged particle distribution ($0 \leq f_i \leq 1$), one can prove that the local equilibrium, $f_i^{eq}$, can be described by Fermi–Dirac statistics (Frisch et al., 1987):

$$f_i^{eq} = \frac{1}{1 + \exp(\alpha + \beta e_i \cdot v)}.$$  

(1.3)

where $\alpha$ and $\beta$ are Lagrange multipliers determined by mass and momentum conservation.

The local averaged particle density, $\rho$, the number density, $n$, and the momentum density, $j$, are defined as follows:

$$\rho(x, t) \equiv m n(x, t) \equiv m \sum_i f_i(x, t),$$

$$j(x, t) \equiv \rho(x, t) v(x, t) \equiv m \sum_i f_i(x, t)e_i,$$  

(1.4)

where $m$ is the mass of one particle (usually equal to 1), and

$$f_i(x, t) = \langle N_i(x, t) \rangle,$$

where "( )" denotes an ensemble average.

In order to obtain the macroscopic hydrodynamic equation, one assumes that, numerically, $\epsilon \sim \frac{1}{L} \sim \frac{1}{T} \ll 1$, where $T$ is the macroscopic characteristic time, $L$ is the macroscopic characteristic length and $\epsilon$ is a small parameter. By taking an
Figure 1.1: The collision rules for the 7-bit lattice-gas automata. The particles have unit mass and unit speed. The left side refers to the state before the collision. The right side refers to the state after collision.

As the ensemble average of (1.1) and assuming molecular chaos, a Taylor expansion gives the continuum version of the kinetic equation

$$\frac{\partial f_i}{\partial t} + e_i \cdot \nabla f_i = \Omega_i,$$

where $\Omega$ is the collision operator obtained by replacing $N_i$ by $f_i$ in (1.2). Using a Chapman–Enskog expansion with the small parameter $\epsilon$ (we will give more details in the next section), it may be shown that the system approximates the following fluid equations (Frisch et al., 1986, 1987):

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho v) = 0,$$
\[
\frac{\partial (\rho \mathbf{v})}{\partial t} + (\mathbf{v} \cdot \nabla) [\rho g(\rho) \mathbf{v}] = -\nabla p + \nu \nabla^2 (\rho \mathbf{v}),
\]
\[p = \frac{1}{2} [\rho - g(\rho) \mathbf{v}^2]. \quad (1.6)
\]

Note that all quantities in (1.6) are dimensionless and \(g(\rho)\) is a function of density which should be unity for the correct Navier–Stokes equation. This causes non–Galilean advection for the velocity field. The incompressible Navier–Stokes equation is recovered only in the low Mach number limit when time, pressure and viscosity are rescaled by the factor, \(g\). Because \(g(\rho)\) depends on density, this rescaling is consistent only for problems which have nearly constant density. Another nonphysical term appears in the equation of state of the lattice–gases where the pressure depends on the local velocity. This will cause some nonphysical compressibility. Thus only small velocity flow can be approximated.

1.3 Lattice–Boltzmann Method

In the lattice–Boltzmann method, space and time are discrete as they are in the lattice–gas method. But instead of using a bit representation for particles, real numbers represent the local ensemble–averaged particle distributions and only kinetic equations for the distributions are solved. This contrasts with lattice–gas models where molecules are represented by bits and the motions of individual particles are followed. The lattice–Boltzmann method ignores particle–particle correlations and often uses simplified collision operators. However, even under these simplifications they provide the correct evolution of the macroscopic quantities. The lattice–Boltzmann method can be viewed to some extent as a finite–difference technique for solving the kinetic equations. The Navier–Stokes equation can be recovered in the long–wavelength and low–frequency limit. The Boltzmann scheme is intermediate between the lattice–gas method and the usual finite–difference algorithms.

As discussed in the last section, the lattice–gas method suffers from several major drawbacks, including a restriction to low Reynolds numbers, a high noise–to–signal ratio, non–Galilean invariance and velocity dependence of the equation of state. One crucial advantage of the continuum description of the lattice–Boltzmann method is that it eliminates most of the noise of the system compared with the lattice–gas method.
In addition, the lattice–Boltzmann method has considerable flexibility in the choice of the local equilibrium particle distribution. In contrast, the Fermi–Dirac equilibrium is the only distribution usually considered for the lattice–gas method. This additional freedom allows us to achieve desired physical properties, such as Galilean invariant convection and a velocity independent equation of state. The advantage of the lattice–Boltzmann method over other finite–difference techniques for obtaining solutions of partial differential equations is that they are fully parallel, resulting in very fast codes. Given the increasing availability of parallel machines, there is a trend to produce numerical codes that exploit the intrinsic features of parallelism. The lattice–Boltzmann methods fulfill these requirements in a very straightforward manner.

The lattice–Boltzmann model was first proposed by McNamara and Zanetti (1988), where they simply replaced $N_i$ by $f_i$ in Equation (1.1) without changing the collision operator and streaming steps. An important refinement of the lattice–Boltzmann method was the recognition that the “exact” collision integral is unnecessarily complex and numerically inefficient if one aims to use it for solving macroscopic equations. Higuera and Jimenez (1989) proposed to linearize the exact Boltzmann collision operator. Expanding on this idea, two groups nearly simultaneously offered the suggestion (Chen, S. et al., 1991e; Qian et al., 1992; Chen, H. et al., 1992) that the exact collision operator can be, in effect, discarded, provided that one adopts a collision operator that leads, in a controllable fashion, to a desired local equilibrium state. By a “desired” equilibrium, it is meant that the situation (i) depends only upon the local fluid variables, which themselves can be computed from the actual values of the local distribution at a point; (ii) leads to the desired macroscopic equations (e.g., the Navier–Stokes equation); and (iii) admits desired additional properties, such as simplicity or removal of nonphysical lattice effects.

As mentioned before, the Boltzmann equation for the hexagonal lattice is constructed by replacing $f_i$, the single–particle distribution, for $N_i$, the particle occupation in Equation (1.1):

$$f_i(x + e_i.t + 1) = f_i(x.t) + \Omega_i(f(x.t)), (i = 0, 1, \ldots, 6). \tag{1.7}$$

where $\Omega_i = \Omega_i(f(x.t))$ is a local collision operator. In the previous section, we saw that Fermi–Dirac statistics are chosen and $f_i$ is restricted to be in a range bounded
by zero and one. For the lattice–Boltzmann method, the particle distribution does not have an upper bound in general. To be consistent with the particle distribution, we require that \( f_i \geq 0 \).

Performing a Taylor expansion in time and space and taking the long–wave and low–frequency limit, we obtain the continuum form of the kinetic equation up to the second order for (1.7):

\[
\frac{\partial f_i}{\partial t} + \mathbf{e}_i \cdot \nabla f_i + \frac{1}{2} \mathbf{e}_i \mathbf{e}_j \cdot \nabla \nabla f_i + \mathbf{e}_i \cdot \nabla \frac{\partial f_i}{\partial t} + \frac{1}{2} \frac{\partial^2 f_i}{\partial t^2} = \Omega_i,
\]

where \( \mathbf{e}_i \mathbf{e}_j \cdot \nabla \nabla f_i \) is the double inner product of two dyads. Now we adopt the following multi–scaling expansion (Frisch et al., 1986). The time and space derivative is expanded as:

\[
\frac{\partial}{\partial t} = \epsilon \frac{\partial}{\partial t_1} + \epsilon^2 \frac{\partial}{\partial t_2},
\]

\[
\frac{\partial}{\partial x} = \epsilon \frac{\partial}{\partial x_1},
\]

where \( \epsilon \) is the expansion parameter as defined in the last section. The above formula implies that the diffusion time scale, \( t_2 \), is much slower than the convection time scale \( t_1 \). Likewise, the one–particle distribution, \( f_i \), is expanded about the local equilibrium distribution,

\[
f_i = f_i^{\text{eq}} + \epsilon f_i^{(1)} + \epsilon^2 f_i^{(2)}.
\]

Inserting \( f_i \) into the collision operator, we have,

\[
\Omega_i(f) = \Omega_i(f^{\text{eq}}) + \epsilon \frac{\partial \Omega_i(f^{\text{eq}})}{\partial f_j} f_j^{(1)} + O(\epsilon^2).
\]

The Chapman–Enskog theory requires \( \Omega_i(f^{\text{eq}}) = 0 \). Neglecting second and higher order terms, we have the linearized form of the collision operator:

\[
\Omega_i(f) = \epsilon M_{ij} f_j^{(1)},
\]

where, \( M_{ij} = \frac{\partial \Omega_i(f^{\text{eq}})}{\partial f_j} \). If we further assume that the local particle distribution relaxes to an equilibrium state at a single rate: \( \frac{\partial f_i}{\partial t} = -\frac{1}{\tau} \delta_{ij} \) with a universal time scale \( \tau \) (the BGK form (Bhatnagar et al., 1954)), we arrive at the following linearized form:

\[
\Omega_i = \frac{-1}{\tau} (f_i - f_i^{\text{eq}}).
\]
Note that we have both \( \sum_i \Omega_i = 0 \) and \( \sum_i e_i \Omega_i = 0 \). The parameter \( \tau \) can be interpreted as the relaxation time due to collisions. The function \( f_i^{eq} \) is the imposed equilibrium distribution for this Boltzmann system. It may be shown from Equations (1.7) and (1.11) that \( f_i \) asymptotically approaches the imposed distribution \( f_i^{eq} \), if the latter is positive everywhere and \( \tau \) is greater than 1/2 (Luo. 1993). In order for the fluid to have Galilean-invariant convection and a pressure which does not depend upon velocity, the following equilibrium distribution, \( f_i^{eq} \), is assumed:

\[
\begin{align*}
f_i^{eq} &= \frac{\rho}{m} \left( \frac{1 - \alpha}{6} + \frac{1}{3} e_i \cdot v + \frac{2}{3} (e_i)_\alpha (e_i)_\beta v_\alpha v_\beta - \frac{1}{6} v^2 \right) \\
f_6^{eq} &= \frac{\rho}{m} [\alpha - v^2].
\end{align*}
\] (1.12)

where \( \alpha \) is a free parameter related to the sound speed as shown below. From (1.8), we can obtain the following equations,

\[
\begin{align*}
\frac{\partial f_i^{eq}}{\partial t_1} + e_i \cdot \nabla f_i^{eq} &= - f_i^{(1)} \\
\frac{\partial f_i^{(1)}}{\partial t_2} + (1 - \frac{1}{2\tau}) \left[ \frac{\partial f_i^{(1)}}{\partial t_1} + e_i \cdot \nabla f_i^{(1)} \right] &= - f_i^{(2)}. \tag{1.13}
\end{align*}
\]

After some simple algebra and using the definition in (1.4), the momentum equation can be written as:

\[
\frac{\partial n v}{\partial t} + \nabla \cdot \tilde{\Pi} = 0,
\]

where the momentum flux density tensor, \( \tilde{\Pi} \), has the form:

\[
\tilde{\Pi}_{\alpha \beta} = \sum_i (e_i)_\alpha (e_i)_\beta [f_i^{eq} + (1 - \frac{1}{2\tau}) f_i^{(1)}].
\]

where \( (e_i)_\alpha \) is the \( \alpha \) component of the velocity vector, \( e_i \). Inserting Equation (1.12) into \( \tilde{\Pi} \) and using the first equation in (1.13), one obtains, to zero order in the small parameter of the Chapman–Enskog expansion,

\[
\tilde{\Pi}^{(0)}_{\alpha \beta} = \sum_i (e_i)_\alpha (e_i)_\beta f_i^{eq}
\]

\[
= 3n \frac{1 - \alpha}{6} \delta_{\alpha \beta} + n v_\alpha v_\beta \tag{1.14}
\]

and

\[
\tilde{\Pi}^{(1)}_{\alpha \beta} = -\tau \left\{ \frac{\partial}{\partial t} \tilde{\Pi}^{(0)}_{\alpha \beta} + \frac{\partial}{\partial x_\gamma} \sum_i (e_i)_\alpha (e_i)_\beta (e_i)_\gamma f_i^{(0)} \right\}. \tag{1.15}
\]
to first order. The final form of the macroscopic equations becomes,

\[
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho v_\beta)}{\partial x_\beta} = 0,
\]

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

\[
+ \frac{\partial}{\partial x_\beta} \left[ \mu \left( \frac{\partial v_\beta}{\partial x_\alpha} + \frac{\partial v_\alpha}{\partial x_\beta} \right) \right],
\]

\[
p = \frac{1 - \alpha}{2} \rho.
\]

(1.16)

In the above equations, \(p\) is the pressure and the sound speed, \(c_s\), is \(\sqrt{\frac{(1-\alpha)}{2}}\). The shear viscosity, \(\mu\), is \(\frac{(r-1)}{8}\) and the bulk viscosity, \(\lambda\), is \(\frac{(r-1/2)(2\alpha-1)}{4}\).

Note that the above equation converges to the exact incompressible Navier–Stokes equations only when the derivatives of the density in the second viscosity term on the right hand side of the equation are small. Since the gradients of the density are \(O(\nu^2)\) (Majda, 1984), the unphysical terms in Equation (1.15) are \(O(\nu^3)\). Thus, although the physics contains compressibility effects, one may come arbitrarily close to solving incompressible flows by reducing the Mach number, \(M = \frac{\nu}{c_s}\).

To solve incompressible fluid flows by traditional numerical methods, such as finite-difference or finite-element, one must deal with a Poisson equation for the pressure term that is induced by the continuum condition and the momentum equation. Here we can see that the solution of the Navier–Stokes equation can be obtained through the lattice–Boltzmann equation in (1.7) and the pressure effects on the momentum equation are controlled by an equation of state. Solution of the Poisson equation is actually avoided by relaxing the incompressibility requirement. It may be argued that CA methods are most closely related to pseudo-compressible algorithms (Ramshaw and Mesina, 1991) for solving incompressible fluid flows.

There may still be some differences between the incompressible Navier–Stokes equation and the macroscopic behavior of the discrete-velocity Boltzmann equations because of the asymptotic nature of the Chapman–Enskog method. These differences could be attributed to higher order terms, such as the Burnett terms, or as small deviations from the above relation for the kinematic viscosity. However, Burnett terms are expected to become negligible as the global Knudsen number, \(K_n = \frac{l}{L}\), becomes small, where \(l\) is the mean free path. Since the Knudsen number is proportional to the
Mach number divided by the Reynolds number, the Burnett terms may be grouped with other "compressibility" effects and should become small as the Mach number approaches zero for a fixed Reynolds number.

It should be mentioned that the numerical implementation for (1.7) is straightforward. At each time step, one calculates a new \( f'_i \) on each lattice: \( f'_i = f_i - \frac{\mu_i f''_i}{r} \), where \( f_i \) and \( f''_i \) are all known functions. Then, \( f'_i \) is advected to a new position, becoming a new \( f_i \). Using the new \( f_i \), the density and velocity can be calculated again.

There are a number of differences between the lattice–Boltzmann method and the lattice–gas method. Without going into detail, the latter approach involves following the dynamics of particles on a lattice. The lattice–gas approach involves only Boolean operations and hence has no numerical roundoff errors and instabilities, in contrast to the floating–point operations in the lattice–Boltzmann method. The difficulty is that the particle–collision rules must be explicitly constructed so as to achieve the desired equilibrium distribution and hydrodynamical properties. In addition, proper statistical averages must be taken to obtain fluid quantities. On the other hand, the lattice–Boltzmann method is similar to an explicit finite–difference scheme, solving the discretized kinetic equation by a Lagrangian upwind scheme (Sterling and Chen, 1993; Skordos, 1993; Ancona, 1994), which is conditionally stable. Stability and accuracy analyses have been provided recently by Sterling and Chen (1993), and by Reider and Sterling (1993), respectively. It has been shown from their analyses that the lattice–Boltzmann methods are second order accurate both in time and space. To ensure numerical stability, the relaxation time should not be less than \( \frac{1}{2} \). (See details in Sterling and Chen (1993) for other parameter dependencies of the stability of lattice–Boltzmann methods).

1.4 Outline of the Following Chapters

Having covered the basics of the lattice–gas and lattice–Boltzmann methods, they will be applied to construct efficient and accurate computer simulations of fluid flow and wave propagation in porous media. The reservoir simulation algorithm based on the lattice–Boltzmann method is addressed in chapter 2, where three lattice–Boltzmann models are presented for single–phase flow, miscible displacement processes, and im-
miscible displacement processes, respectively. In chapter 3 the lattice–Boltzmann approach is developed for simulations of seismic wave propagation in inhomogeneous media. While it is natural to extend the fluid–based lattice–Boltzmann model to simulation of acoustic waves, the lattice–Boltzmann model for elastic waves is motivated by the similarity between Navier–Stokes equation and the elastic wave equation. Material in Chapter 4 describes the applications of CA methods to microscopic simulations of rocks, particularly, the lattice–gas method to rock permeability calculations and lattice–Boltzmann acoustic model to rock attenuation investigations. Finally summaries of present research and recommendations for further investigation are presented in Chapter 5.
Chapter 2

Lattice Boltzmann Simulations of Fluid Flow in Porous Media

The simulation of multiphase flow in porous media is of great importance, especially in petroleum reservoir engineering where the results of reservoir simulation may lead to large capital investments and may be a prime factor in estimating the amount of oil (or gas) recovery. The purpose of reservoir simulation is to optimize profits from a reservoir by finding the best strategy for placement of wells, injection and production flow rates, and choice of injectants. An accurate analysis of a reservoir would require understanding of its geology and resident fluids, together with an accurate model of the flow and interactions of these fluids under the influence of injection and production wells. The flow models involve coupled systems of nonlinear partial differential equations that cannot be solved exactly by analytical means, so simulations must use numerical approximations on computers.

2.1 Background on Reservoir Simulation

2.1.1 Physical models

A petroleum reservoir is a heterogenous porous medium, whose permeability and porosity vary on a wide range of length scales. In this medium resides a complex collection of chemical fluid species, usually called components. These include water and hydrocarbarbons, such as methane, ethane, propane, and so on. The components mix
to form fluid phases; these are the flowing entities, each of which has its own pressure, density, and viscosity. When multiple phases are present, there is a force of surface tension at the interface between them, leading to a difference between the phase pressures known as capillary pressure. Under most circumstances, there are three phases: a water phase, consisting mostly of water with possibly some dissolved hydrocarbons, a gas phase with mostly light hydrocarbons and possibly some volatilized heavy hydrocarbons and water vapor, and an oil phase, with mostly heavy hydrocarbons and some dissolved light hydrocarbons and possibly water. The pressure and the amounts of the various components present determine how the components partition themselves among the phases; this mass transfer is extremely important because different phases have very different flow properties.

The processes by which oil is extracted from a reservoir are commonly broken down into primary, secondary, and tertiary recovery. We will discuss these from the point of view of the difficulties in modeling them. In primary recovery, production wells are opened and made to flow, usually at specified rates that change discontinuously from time to time. When a rate changes, a transient pulse is introduced into the reservoir pressure field around the corresponding well. Typically, as time elapses, this pulse dies out and a new smooth pressure field evolves. The pressure controls the fluid flow; phases flow toward production wells according to their respective mobilities, but no fluid is injected and no significant displacement occurs. Mathematically, this is a diffuse, parabolic process that presents few problems to standard solution techniques.

Primary recovery produces, on the average, about one third of the original oil in place in a reservoir. In secondary recovery, or waterflooding, some of the remaining oil is produced by injecting water at certain wells in order to displace oil to other wells. This creates a moving displacement front, which is harder for solution methods to represent accurately. However, water continues to be injected for many years or perhaps even decades, so that the process goes on long after the front has broken through at production wells. Except in rare instances, water is thermodynamically inert; temporary errors in its saturation have little if any effect on hydrocarbon phase behavior and the resulting transport of components in phases. Thus, any simulation errors tend to cancel themselves out over time. Ultimate recovery is mainly a function of sweep efficiency (the fraction of the reservoir swept by water), residual oil saturation
(the saturation below which oil cannot flow), and capillary pressure, the force that traps oil in pores swept by water. Secondary recovery typically leaves a bit more than half of the original oil behind.

This oil is the target of tertiary recovery, also called enhanced oil recovery (EOR), which is much more difficult to model. EOR processes are usually divided into three categories—miscible, chemical, and thermal (Broome et al., 1986). Miscible processes inject a solvent of carbon dioxide, nitrogen, or hydrocarbons to mix with reservoir oil, either upon initial contact ("first-contact miscibility") or, more commonly, after exchanges of hydrocarbon components between the injectant and the oil ("multiple-contact miscibility"). When miscibility is achieved, there is no surface tension between the displacing injectant and the oil (they flow together as one phase). So in principle it is possible to recover all of the oil by displacement. In practice, this does not occur. The injectant is too expensive to use indiscriminately, so only a slug that would fill some small fraction of the reservoir (often 5% to 15%) is injected. This is followed by a cheaper, immiscible fluid that can be injected continuously, such as water. As the slug moves through the reservoir, permeability heterogeneities cause it to prefer certain flow paths and diffusive effects reduce its peak concentration. Because the injectant is normally less viscous than the oil, the displacement front is unstable, and a phenomenon called "viscous fingering" causes the injectant to make finger-like channels into the oil, by passing much of the oil outside these fingers. Eventually the slug can be expected to break up and lose its effectiveness. Phase behavior (miscibility or the lack thereof) is crucial in these processes, and it is quite sensitive to the pressure and the evolving compositions of the slug and the oil.

Chemical flooding injects a polymer, surfactant, or alkaline solution. The purpose of polymers is to increase the viscosity of injected water so that the mobility ratio of injectant to oil will be reduced. This mitigates viscous fingering and improves the sweep efficiency of the displacement, with less oil being bypassed. A surfactant, which is like a detergent, is intended to lower the surface tension between injectant and oil. Unlike a miscible flood, surface tension is not reduced to zero, but is made low enough so that much more oil can be "washed" out of the porous rock than would be possible without the surfactant. Polymer may be added to the surfactant solution for the sake of mobility control. Alkaline solutions, also with the possible addition of polymer.
perform similarly, except that they react with the constituent of crude oil to produce surfactants, which then act to lower surface tension. The amount of mobility control or surface-tension reduction depends strongly on the evolving chemical concentration and oil composition, and the amount of bypassed or trapped oil in turn depends strongly on mobility and surface tension.

Thermal processes include cyclic ("huff-n-puff") or continuous steam injection and in situ combustion. In any of these, the goal is to raise the temperature of the reservoir, lowering the viscosity of the resident oil and changing other properties to improve recovery. In cycling, steam is injected into a well which is then shut in so that the heat will diffuse; the well is then reopened as a producer, and the entire process is repeated. This has the flavor of primary recovery. Continuous injection, or steamflooding, instead displaces oil from an injector to a producer, and can be viewed as waterflooding (secondary recovery) with heat. Oxygen ahead of the combustion front reacts with oil to produce coke, which is the actual combustion fuel. The combustion products heat and displace the oil to production wells. The front is narrow, and proper conditions for complex reactions in and around the front must be maintained for the process to work.

Aside from steam injection, all of the EOR processes just described share the property that there is a narrow moving zone in which a crucial variable, either concentration or temperature, varies rapidly. For faithful modeling of the physics, this variable must be approximated accurately in the narrow zone. In miscible flooding, miscibility itself is sensitive to peak solvent concentration, and viscous fingering, which determines sweep efficiency, is governed by the interactions of mobility ratio, heterogeneities, and diffusive effects that depend on the concentration profile of the front as well as its location. Viscous fingering is likewise important in chemical flooding, and the peak concentration of the injected chemical determines the amount of mobility control (for polymer) or surface-tension reduction (for surfactant or alkali) and hence the effectiveness of the process. Peak temperature and concentrations of resulting substances determine whether in situ combustion will continue or cease, and how effectively it will reduce oil viscosity.
2.1.2 Derivation of simulator equations

First, let us introduce some very basic reservoir engineering. Permeability, the conductive property of a porous material to fluid flow may be defined by Darcy’s law:

\[
\mathbf{u} = -\frac{\mathbf{K}}{\mu} \cdot \nabla p.
\]  

(2.1)

For a single fluid, Darcy’s law states that the volumetric rate of flow per unit area, \(\mathbf{u}\), which has units of velocity, is proportional to the pressure drop per unit length, \(\nabla p\), and inversely proportional to the viscosity of the fluid, \(\mu\). The permeability tensor, \(\mathbf{K}\), is simply the constant of proportionality in the flow direction. It is a property of the porous rock, and it can be a function of position.

Another important property of the porous rock is its porosity, \(\phi\), which is the ratio of void volume to total volume. It can also be a function of position.

Mass flux is obtained by multiplying (2.1) by the density of the fluid, \(\gamma\). The effect of gravity is included by adding the term \(g\gamma \nabla h\) to the pressure gradient, where \(g\) is the acceleration due to gravity, and \(h\) is the elevation. Thus

\[
\gamma \mathbf{u} = -\frac{\gamma \mathbf{K}}{\mu} \cdot (\nabla p - \gamma g \nabla h).
\]  

(2.2)

However, we are almost always interested in the simultaneous flow of several fluids, such as the displacement of oil by water. In that case, within any one pore we might get a piston-like displacement. But on any scale larger than pore size, the water penetrates into the oil zone, and both fluids appear to be flowing in the same place at the same time. Usually, in fact, we are interested in the simultaneous flow of three fluids: oil, gas, and water.

The saturation. \(S_l\), of each phase. \(l\), is the fraction of the void volume occupied by that phase. When several fluids try to flow together, they get in each other’s way. The permeability of the porous rock, \(\mathbf{K}\), has to be multiplied by the relative permeability, \(k_{rl}\), to get the flow for each phase. \(l\). Thus,

\[
\gamma_l \mathbf{u}_l = -\frac{\gamma_l \mathbf{K} k_{rl}}{\mu_l} \cdot (\nabla p_l - \gamma_l g \nabla h)
\]  

(2.3)

where \(l = \text{water, oil or gas}\). Relative permeability is believed to be an increasing function of saturation, since the higher the saturation of each phase, the easier it is
to flow. The relative permeability functions are in practice taken to be correlations of experimentally derived values: typical curves for \( k_{rl} \) in a two phase system are shown in Figure 2.1, where \( w \) denotes the "wetting" phase and \( n \) the "nonwetting" phase (in a oil–water system, water is the wetting and oil the nonwetting phase).

Another phenomenon associated with multiphase flow is the capillary pressure. Because the sand particles usually attract water more than they attract oil, the pressure in the oil will be higher than the pressure in the water; this difference in pressure is called the oil–water capillary pressure, \( p_{c_{ow}} \), and it is a function of the water saturation.

\[
p_{c_{ow}} = p_{oil} - p_{water} = p_{c_{ow}}(S_w)
\]  

(2.4)

Similarly, the difference between the gas and oil pressures is the gas–oil capillary pressure, a function of the gas saturation.

\[
p_{c_{go}} = p_{gas} - p_{oil} = p_{c_{go}}(S_g)
\]  

(2.5)

The saturation \( S \) may be derived from a knowledge of a \( p_c \) vs \( S \) curve, such as that given in Figure 2.2 (derived experimentally for the case when wetting is the driving (imbibition) or displacing (drainage) fluid).

Now we consider the fact that each phase, oil, water, or gas, is not necessarily a single chemical species, but may contain more than one component, such as methane, ethane, butane, etc. It may also contain non-hydrocarbons such as water, \( CO_2 \), nitrogen, or even a surfactant. Within each phase, \( l \), the concentration of each component, \( i \), is given by the mass fraction, \( C_{li} \), so that the transport of that component in that phase is given by the equation.

\[
C_{li} \gamma_i \mathbf{u}_l = -C_{li} \frac{\gamma_i K_{xi}}{\mu_l} \left( \nabla p_l - \gamma_i g \nabla h \right) - \mathbf{D} \cdot \nabla C_{li}.
\]  

(2.6)

where \( l \) = water, oil or gas, and \( i = CH_4, C_2H_6, \ldots, H_2O, CO_2, N_2 \), or surfactant. The first term on the right of (2.6) is the transport due to convection, as given by Darcy's law. The second term is the additional transport due to diffusion or dispersion, where \( \mathbf{D} \) is the dispersion tensor.

Finally, we have the conservation law, which states that the mass of each component is conserved.

\[
\sum_l \frac{\partial (\sigma S_i \gamma_i C_{li})}{\partial t} = -\sum_l \nabla \cdot [C_{li} \gamma_i \mathbf{u}_l] + q_i.
\]  

(2.7)
Figure 2.1: Typical relative permeability curves for oil \( k_r \) and water \( k_{rw} \) as a function of water saturation \( S_w \). The value of \( S_w \) at which water starts to flow is called the critical saturation \( S_{wc} \). The saturation \( S_{nc} \), at which the displaced phase ceases to flow is called the residual saturation.

Figure 2.2: Typical capillary pressure versus water saturation and its change (drainage or imbibition) curves. The value \( P_c \) which is necessary to start displacement is called "threshold pressure" (Bear, 1972). The value of saturation at which the wetting phase no longer can be displaced by applying a pressure gradient is called "irreducible saturation".
Note the summation over all the phases, $l$. Here $q_l$ is a source–sink term that accounts for injection or production at the wells.

Combining the conservation equations with the transport equations gives the following system of differential equations, one equation for each component.

$$\sum_l \frac{\partial (\phi S_l C_{il})}{\partial t} = \sum_l \nabla \cdot \left[ \frac{C_{il} \gamma_l \tilde{K}_{il}}{\mu_i} (\nabla p_l - \gamma_l g \nabla h) \right] + \sum_l \nabla \cdot \left[ \tilde{D} \cdot \nabla C_{il} \right] + q_l. \quad (2.8)$$

These variables are also coupled together by additional relations, which are discussed below.

For an isothermal displacement, this equation is the whole story. If we were to consider thermal processes, such as steam flooding or in situ combustion, we would have to include another equation for the energy balance. It is true that thermal processes are some of the most important methods for enhanced oil recovery. Still, in the current state of the art, most reservoir simulation deals with isothermal displacement. So, we will concentrate on the isothermal case.

While (2.8) is the only differential equation we need to consider now, we need some additional relations to complete the mathematical specification. These are summarized in Table 2.1. First, the saturations of the various phases must add up to one. Within each phase, the mass fractions of the various components must add up to one. We need to incorporate the assumption of thermodynamic equilibrium, which accounts for the way in which the various components distribute themselves among the phases. The calculations for determining this distribution, such as the Peng–Robinson equation of state (Peng and Robinson. 1976. 1977), is usually referred to as the V.L.E. calculation for vapor–liquid equilibrium. Of course, it can be more general than just involving vapor and liquid phases.

This distribution can be represented in a general way as follows. Let $m_i$ be the total mass of each component in the total pore volume, $V_T$. Then.

$$m_i = V_T \sum_l C_{il} \gamma_l S_l.$$  

For a given pressure, temperature, and collection of $m_i$'s, the V.L.E. calculation yields the total volume, the volume of each phase, the concentration of each component in each phase, as well as the density and viscosity of each phase. This is indicated in the third line of Table 2.1.
\[ \sum_i S_i = 1, \]
\[ \sum_i C_i = 1. \]
\[
\begin{align*}
&\text{p. T. } m_i \xrightarrow{\text{V.L.E.}} V_T, V_i, C_i, \gamma_i, \mu_i, \\
&S_i = \frac{V_i}{V_T}, \\
&k_{ri} = k_{ri}(S, x, C), \\
p_{cp} = p_{cp}(S, x, C), \\
&\phi = \phi(x, p), \\
&\bar{K} = \bar{K}(x).
\end{align*}
\]

Table 2.1: Auxiliary relations for reservoir simulators.

Continuing in Table 2.1, we recall that the ratio of phase volume to total volume is the saturation of that phase. Relative permeabilities and capillary pressures are considered to be empirical functions of saturation, and they may also be functions of position. In addition, relative permeabilities and capillary pressures may also be functions of concentrations. Rock porosity, \( \phi \), is a function of position, and can also be a function of pressure, since the rock may have some compressibility. Finally, the rock permeability, \( \bar{K} \), is some function of position.

What we have just described is for a full multicomponent, multiphase, displacement, which, in reservoir engineering, is usually referred to as compositional simulation. It allows for the possibility that each component can exist in any or all of the phases. Such a complete description is what we need for many enhanced recovery processes. It is, of course, very expensive to compute.

An important simplification of the V.L.E. is the so-called “black-oil” model. It assumes that the aqueous phase contains only water, and that the hydrocarbon vapor phase contains only one component, called “gas”. The hydrocarbon liquid phase is assumed to contain two components: oil without any dissolved gas, which is called “dead oil” or “black oil” (hence, the name) and gas, which can transfer back and forth between the hydrocarbon liquid and vapor phases. Because the hydrocarbon
liquid–vapor system has only two components, the oil concentration is a function of pressure only and simplified empirical functions of pressure result. If \( R_{go}(p) \) is the dissolved gas ratio, equal to the mass of gas dissolved in a unit mass of dead oil, the following substitutions for concentrations become:

\[
C_{ww} = 1 \quad C_{ow} = 0 \quad C_{gw} = 0
\]

\[
C_{wo} = 0 \quad C_{oo} = \frac{1}{1 + R_{so}} \quad C_{go} = \frac{R_{so}}{1 + R_{so}}
\]

\[
C_{wg} = 0 \quad C_{og} = 0 \quad C_{gg} = 1.
\]

Then the system of differential equation (2.8) reduces to the following three equations (Peaceman, 1977),

\[
\frac{\partial}{\partial t} \left[ \frac{\phi S_g}{B_g} \right] + \frac{\partial}{\partial t} \left[ \frac{\phi R_{so} S_o}{B_o} \right] = \nabla \cdot \left[ \frac{\tilde{K} k_{rg}}{B_g \mu_g^*} \cdot (\nabla p_g + \gamma_g g \nabla h) \right] + \nabla \cdot \left[ \frac{R_{so} \tilde{K} k_{ro}}{B_o \mu_o} \cdot (\nabla p_o + \gamma_o g \nabla h) \right] + q_g; \quad (2.9)
\]

\[
\frac{\partial}{\partial t} \left[ \frac{\phi S_o}{B_o} \right] = \nabla \cdot \left[ \frac{\tilde{K} k_{ro}}{B_o \mu_o} \cdot (\nabla p_o + \gamma_o g \nabla h) \right] + q_o; \quad (2.10)
\]

\[
\frac{\partial}{\partial t} \left[ \frac{\phi S_w}{B_w} \right] = \nabla \cdot \left[ \frac{\tilde{K} k_{rw}}{B_w \mu_w^*} \cdot (\nabla p_w + \gamma_w g \nabla h) \right] + q_w. \quad (2.11)
\]

Equation (2.9) is a gas balance: it includes the transport of gas in both the vapor and liquid phases. Equation (2.10) is a balance on the oil, which is transported only in the liquid phase. Equation (2.11) is a balance on the water.

Black oil simulators can solve some quite realistic field problems, since they account for the three-phase flow of oil, gas, and water, for compressibility, and, most importantly, for the presence of dissolved gas in the oil. Because of this, they have become the work–horse of the reservoir industry, and are in routine use by reservoir engineers. However, black–oil simulators are not sufficiently realistic for predicting the performance of most enhanced recovery projects. These projects usually involve more complex phase behavior that requires anywhere from four to twenty components to model it realistically. For such projects, fully-compositional models are needed. In addition to being very expensive to compute, the mathematical structure of a fully compositional system is very poorly understood.

Research on numerical methods for reservoir simulation is usually carried out on model problems that avoid the complexities involved in simulating real field problems.
which exhibit the same numerical difficulties. Of them, two most popular models are the miscible displacement problem and immiscible displacement problem, which we will discuss in detail in Sections 2.3 and 2.4, respectively. The assumptions under the immiscible displacement are that there are only two phases, and there is no mass transfer between the phases. This is equivalent to saying that each phase consists of only one component. Miscible displacement is an important simplification of the fully-compositional model where the components mix together and form a single phase.

2.1.3 Numerical methods

The most popular numerical approach to the simulation of large reservoir systems is the method of finite differences. There are several practical reasons for this popularity. Finite difference methods are conceptually straightforward. The fundamental concepts are readily understood and do not require advanced training in applied mathematics. Moreover, due to their extensive history, they boast a firm theoretical foundation. In addition, because of the form and algebraic simplicity of the equations arising from difference approximations, several clever algorithms have been developed for their solution. Two excellent monographs on the application of finite difference theory to reservoir simulation (Aziz and Settari, 1979; Peaceman, 1977) are important references in this topical area.

Motivated by the unsatisfactory finite difference solutions obtained for the convective–diffusive transport equation, Price et al. (1968) introduced Galerkin’s finite element concepts into the reservoir simulation literature. Whereas solutions of high accuracy were generally achieved, it was also conceded that the Galerkin finite element schemes were, for the most part, noncompetitive with finite difference algorithms because of their computational inefficiency. Some works (i.e., Young, 1981) have sought to change this prognosis.

Recognizing that the convection–dominated transport equation behaves as a first-order rather than a second-order partial differential equation, Garder et al. (1964) introduced the method of characteristics as an appropriate solution methodology. This approach to solving partial differential equations is known to be effective for equations of hyperbolic type (Bratredt et al., 1992). The practical difficulties associated with the utilization of the method of characteristics are evident to anyone who attempts
to simulate a field situation. The method involves tracking mathematical particles as they move along characteristic curves. The programming sophistication required to generate an efficient yet generally applicable code is considerable. Moreover, the method does not have the same degree of mathematical rigor as that identified with other solution procedures.

It is evident that each of the three generally recognized reservoir simulation methodologies has its own advantages and disadvantages. The finite difference approach is simple in concept and implementation: the finite element approach provides a flexible mesh geometry and can be more accurate for certain operators; finally, the method of characteristics can be effectively employed to simulate convection-dominated transport problems. However, the pressure equation is almost elliptic in character and this precludes the use of explicit numerical schemes. The standard numerical methods for reservoir simulation are, accordingly, at least partially implicit (Peaceman. 1977; Aziz and Settari. 1979), corresponding to the solution of the pressure equation or some equivalent thereof. Consequently, the computation is dominated by linear-equation solution and, unfortunately, the best methods in common use involve recursive preconditioners that do not vectorize or parallelize well. The lattice Boltzmann method is, however, well-suited for vector and parallel processing and is inherently simple and easy to implement. In addition, it does not depend on a belief in the previously described engineering theory.

2.2 Single-phase Flow

2.2.1 Darcy's law

Processes taking place in porous media could, in principle, be studied at either microscopic or macroscopic levels. From the microscopic viewpoint, the temporal and spatial distributions that describe the considered process could be derived by solving the hydrodynamics equations in the pore space, subject to the appropriate initial and boundary conditions. Among these computer simulation techniques are lattice gas automata methods (Frisch et al.. 1986) which, in the context of fluid flow problems, are the discrete solutions of the Navier-Stokes equations. In the past few years, lat-
tice gas automata methods, with their extension to lattice Boltzmann methods have been used by many authors (Rothman, 1988; Chen, S. et al., 1991a) for investigating various flow phenomena in porous media.

However, in a real physical situation, a porous medium represents an infinitude of pore shapes and sizes. This complexity of the configuration of the boundary surface renders hopeless any attempt to follow this procedure as a method of solving practical problems. Moreover, even if we could solve them in the pore size, the solutions would be of no practical value as no instrument is available for measuring values of the considered variables in the studied porous medium domain in order to compare them with such solutions. In an attempt to circumvent these fundamental difficulties, and in response to the practical needs of industry, a semiempirical macroscopic description of fluid flow through porous media has usually been used. In this approach, Darcy’s law is used in place of the Navier-Stokes equation. Darcy’s law is a typical macroscopic empirical law, which circumvents the need to know the exact configuration of boundary surface and enables the description of phenomena in terms of measurable quantities. It states that in a porous medium, the velocity of the fluid in proportional to the gradient of pressure which drives it. The expression of the law is

\[ u = -\frac{k}{\mu} \nabla p \]  

(2.12)

where \( k \) is defined as the medium permeability, and \( \mu \) is the viscosity. Previous attempts at developing a model which can directly simulate Darcy’s law have been made by using lattice gas methods with introduction of damping scatters (Balasubramanian et al., 1987; Somers and Rem. 1991b). Due to their Boolean nature, the correct Darcy type flow is only obtained if the percentage of scatters is small (less than 5%).

Our objective in this section is to introduce a lattice Boltzmann model that can simulate flow though porous media according to Darcy’s law instead of the Navier-Stokes equation. Specifically, we add a damping term to the collision operator of lattice Boltzmann models that makes the momentum dissipate due to fluid particles hitting the solid of the porous medium. This addition results in a momentum proportional to the gradient of the pressure which drives it according to Darcy’s law while mass is conserved. In addition, the model makes provision for a compressible fluid through a compressible medium by assuming that (i) both fluid and medium are elastic bodies
following Hook's law, i.e.,

\[ \gamma = \gamma_0 + c_f(p - p_0), \tag{2.13} \]
\[ \phi = \phi_0 + c_R(p - p_0), \tag{2.14} \]

where \( \gamma \) is the density of the fluid and \( \phi \) the porosity of the solid at pressure \( p \), \( \gamma_0 \) and \( \phi_0 \) the density and porosity at the reference pressure \( p_0 \), \( c_f \) and \( c_R \) are fluid density and porosity compressibility coefficients, respectively, (assumed to be constant); and that (ii) the permeability of the medium does not change during compression.

### 2.2.2 Numerical model

The starting point of the lattice Boltzmann method is the kinetic equation for the velocity distribution function. For computational efficiency, our model consists of particles moving along the main directions of a hypercubic lattice (a square lattice in two-dimensions or a cubic lattice in three-dimensions) due to only linear momentum flux involved in Darcy’s law. If the nonnegative, real number \( f_i(x, t) \) is the particle population at lattice node \( x \) and discrete time \( t \), moving along direction \( i \), the lattice Boltzmann equation for this model can be written as

\[ f_i(x + e_i, t + 1) = f_i(x, t) + \Omega_i(x, t), \quad i = 1, \ldots, N, \tag{2.15} \]

where \( \Omega_i \) is the collision operator which represents the rate of change of \( f_i \) due to collisions, and \( N \) is the number of degrees of freedom or the number of main directions of a hypercubic lattice (4 for a square lattice and 6 for a cubic lattice). For simplicity, we will discuss a two dimensional fluid model in what follows. The extension of this model to a three dimensional one is straightforward.

The microscopic dynamics associated with Equation (2.15) can be viewed as a two step process: free streaming and collision. During the free streaming step, \( f_i(x) \) is replaced by \( f_i(x + e_i) \). Thus, each site exchanges mass with its neighbours, i.e. sites connected by lattice vector \( e_i \). In the collision, to preserve the advantage of doing parallel computing, we add a damping term \( \Omega^d_i \), which contains only local information and satisfies the momentum constraints at each site, to the BGK relaxation term (Qian et al., 1992) of the Boltzmann equation. That is,

\[ \Omega_i = \frac{1}{\tau}(f_i^* - f_i) + \Omega_i^d. \tag{2.16} \]
Here the distribution $f_i$ and its local equilibrium state $f_i^{eq}$ correspond to the identical value of local density $\rho$ and velocity $v$, and $f_i^{eq}$ can be chosen to have the form,

$$f_i^{eq} = \frac{\rho}{4} (1 + 2e_i \cdot v).$$  

(2.17)

The constant $\tau$ is the characteristic relaxation time, which is chosen to achieve a desired kinetic viscosity $\nu$ according to

$$\nu = \frac{1}{4} (\tau - \frac{1}{2}).$$  

(2.18)

For Darcy type flow in porous media, velocity magnitudes are generally sufficiently low, and characteristic pore dimensions sufficiently minuscule to render the relevant Reynolds number small compared with unity. Thus, the inertial effects generally can be ignored and $\tau$ may be set close to one half.

The mass and momentum of the fluid at a site are obtained by using the following sums over all velocity directions.

$$\rho = \sum_i f_i = \sum_i f_i^{eq},$$  

(2.19)

$$\rho v = \sum_i f_i e_i = \sum_i f_i^{eq} e_i.$$  

(2.20)

Here, the bulk density $\rho$ represents the mass of the fluid per unit volume of porous medium while the true density of the fluid $\gamma$ represents the mass of the fluid per unit volume of the fluid. These two densities are related by

$$\rho = \phi \gamma$$  

(2.21)

in which $\phi$ is the porosity defined as the fraction of the pore in the medium.

The damping term of the collision operator results from the presence of extrinsic momentum dissipation due to flow through the porous medium according to Darcy's law (2.12). Motivated by that given in Balasubramanian et al.'s (1987) paper, the bouncing back of any particle either into or out of direction $i$, after hitting scatterers at a given site, can be described as:

$$\Omega_i^d = \frac{b}{4k + b} (f_{i+2} - f_i),$$  

(2.22)

where

$$b = \mu (\phi e_f + \gamma c_R)/\gamma.$$  

(2.23)
Note that when $\phi = 1$ and $k \gg 1$, $\Omega_i^d = 0$. Thus, this damping term only affect the fluid flow through porous media.

To derive the hydrodynamic equations, we take the long-wavelength low-frequency limit of Equation (2.15), to obtain

$$
\frac{\partial f_i}{\partial t} + e_i \cdot \nabla f_i + \frac{1}{2} e_i e_i : \nabla \nabla f_i = \Omega_i .
$$

(2.24)

Using the definitions (2.16) and (2.22) for the collision operator, Equation (2.24) leads, after summation, to the mass conservation,

$$
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 ,
$$

(2.25)

and, after multiplication with $e_i$ and summation, to the following momentum equation.

$$
\frac{\partial \rho \mathbf{v}}{\partial t} = - \frac{1}{2} \nabla \rho - \frac{2b}{4k + b} \rho \mathbf{v} .
$$

(2.26)

For a "slow" flow, like Darcy flow in porous media, the convective terms are generally negligible. Thus, Equation (2.26) reduces to

$$
\nabla \rho = - \frac{\mu}{k + \frac{b}{4}} \frac{\rho \mathbf{v}}{\gamma} .
$$

(2.27)

Since the traditional form is given in terms of the volume velocity, $\mathbf{u}$, defined as

$$
\mathbf{u} = \phi \mathbf{v} ,
$$

(2.28)

the final mass and momentum equations may be expressed as

$$
\frac{\partial \phi \gamma}{\partial t} + \nabla \cdot (\gamma \mathbf{u}) = 0 ,
$$

(2.29)

$$
\mathbf{u} = - \frac{(k + \frac{b}{4})}{\mu} \nabla \rho .
$$

(2.30)

Here, we do not have the exact Darcy's law (2.12) because the actual particle current is not equal to $\rho \mathbf{v}$ due to discretization of the lattice. This difference usually appears as a correction to the transport coefficients due to the discretization of space (Henon, 1987).

So far, we only have discussed compressible fluid flow. Strictly speaking, lattice gas methods and their extensions to lattice Boltzmann methods should be restricted
Figure 2.3: The numerical pressure distribution of a steady-state flow along an inhomogeneous channel with three different permeabilities of 1.0, 0.1 and 2.0 lattice units, computed with $\gamma u = 0.0125$, $\mu = 1$ and $\gamma = 3.2$.

to solving compressible fluid flows. However, the incompressible limit theory of the lattice gas method and its numerical simulations predicted and demonstrated that lattice gas studies at low Mach number produce results comparable with those of the incompressible Navier-Stokes equations for a wide variety of problems and with very small numerical errors. This approach has much in common with the explicit “penalty” or “pseudocompressibility” method of solving incompressible fluid flows. Specifically, to deal with incompressible fluid flow in our model, an artificial kind of small compressibility is required by setting a finite value of $c_f$. The examples in this thesis will show that this method has very small numerical errors.

2.2.3 Simulation and validation

To qualitatively verify that our model is indeed simulating hydrodynamics of fluids in porous media correctly, we will show three examples of both compressible and incompressible fluid flows through one-dimensional and two-dimensional porous media.
Figure 2.4: The theoretical prediction (solid line) and numerical solutions (plus sign, asterisk and diamond) of linear non-steady state flow for different combination of the fluid compressibility and medium compressibility.

The first numerical test is the steady state flow in one-dimension, where the channel is divided into three segments with different permeabilities of $k = 1.0, 0.1, 2.0$ lattice units. The boundary conditions for this one-dimensional example were $p = 0$ initially, and $\gamma u = 0.0125$ injected at $x = 0$ and $\gamma u = 0.0125$ produced at $x = L$ with $L = 100$ lattice units. Since this is an incompressible fluid flow case, an artificial compressibility $c_f = 0.2$ lattice unit was used as required for our lattice Boltzmann algorithm. From the simulated pressure profiles in Figure 2.3 and with $\mu = 1$ and $\gamma = 3.2$, we can calculate the permeabilities, which agree well with the prescribed values.

The second numerical test is an unsteady state flow in linear approximation, where Equations (2.14) and (2.14) were used as the general density and porosity functions of the pressure. By combining Equations (2.12) and (2.29), we can write the governing differential equation as follows

$$a^2 \frac{\partial^2 p(x, t)}{\partial^2 x} = \frac{\partial p(x, t)}{\partial t},$$

(2.31)
Figure 2.5: The pressure distribution for a two-dimensional steady state flow computed by using the analytical method.

Figure 2.6: The pressure distribution for a two-dimensional steady state flow computed by using the lattice Boltzmann method.
\[
a^2 = \frac{k\gamma_0}{\mu (\phi_0 c_f + \gamma_0 c_R)} \quad (2.32)
\]
with boundary conditions
\[
\begin{align*}
  p(0, t) &= p_0, \quad t > 0 \\
  p(L, t) &= p_1, \quad t > 0 \\
  p(x, 0) &= p_0, \quad 0 < x < L.
\end{align*}
\quad (2.33)
\]

The solutions of this simple flow are present in most standard texts (i.e., Scheidegger, 1974). In order to give a series of "standard" solutions, it is convenient to introduce the following dimensionless parameters,
\[
\epsilon = \frac{x}{L}, \quad F = 2 \frac{a^2}{L^2} t, \quad W = \frac{p_0 - p}{\epsilon (p_0 - p_1)}. \quad (2.34)
\]

With these notations, the solution of the problem becomes
\[
W(\epsilon, F) = 1 - \frac{2}{\pi \epsilon} \sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{n} \exp\left(-\frac{n^2 \pi^2 F}{2}\right) \sin(n \pi \epsilon) \quad (2.35)
\]
where \( n \) is an integer. Each term in the series is a particular solution as one can easily verify by direct differentiation and substitution. It should be noted that as \( n \) increases, the terms in the series tend to zero rapidly. In Figure 2.4 we present the analytical prediction and direct numerical simulation with \( k/\mu = 1.25 \) and \( \phi_0 = 0.5 \) for different combinations of fluid compressibility and rock compressibility, where the solid line represents the theoretical prediction with \( a^2 = 0.25 \), the plus sign represents simulation with \( c_f/\gamma_0 = 8.0 \) and \( c_R = 1.0 \), the asterisk with \( c_f/\gamma_0 = 10.0 \) and \( c_R = 0.0 \) and the diamond with \( c_f/\gamma_0 = 0.0 \) and \( c_R = 5.0 \). As seen, the agreements are excellent.

The last numerical test is a two-dimensional well-pumping experiment in a homogeneous square reservoir. Here, two injectors with flow rate \( q \) were located in the lower left corner and upper right corner, respectively, and two producers with the same flow rate in the lower right corner and upper left corner, respectively. The pressure distribution for this problem can be obtained by using the so-called "method of images" as popular in the study of electrical potential theory. Briefly, in order to maintain a strict no-flow condition at the out boundary requires the placement of an infinite grid of virtual or image wells, each well producing or injecting at the same rate as the real
wells within the boundary. The steady state solution for this complex system can be expressed as,
\[ p(x, y) = \frac{\mu}{4\pi} \sum_{i=1}^{\infty} q_i \ln \frac{(x-x_i)^2 + (y-y_i)^2}{x^2 + y^2}. \] (2.36)
where \( q_i \) is the flow rate of the \( i^{th} \) well at \((x_i, y_i)\). The infinite summation is an example of superposition in space of the basic point sink solution of the infinite array of the well system. The most striking verification of the accuracy of our model for this particular problem, perhaps, is found in the direct comparison of the contour plots of the simulation pressure distribution and analytical pressure distribution as shown in Figures 2.5 and 2.6, respectively. We see that the pressure distribution is extremely similar in the two cases except for a perceptible level of background in the analytical solution. The background noise is present because of the omission of high-order terms in the summation in Equation 2.36, thereby decreasing the effective precision of the numerical calculations.

2.2.4 Concluding remarks

A lattice Boltzmann model has been developed to model hydrodynamics in porous media according to the macroscopic, empirical Darcy's law. It is an extension of the lattice gas model proposed by Balasubramanian et al. The current model allows simulation of a wide range of permeabilities for both compressible and incompressible fluid flows. The simulation results for several, one-dimensional or two-dimensional, steady state or unsteady state flows are shown to be in good agreement with analytical solutions. It should be pointed out that the single-phase flow in porous media can be formulated in terms of a nonlinear diffusion equation for compressible fluids (Brieger and Bonomi. 1991). However, the model proposed here is in parallel to the theoretical derivation of Darcy's law (Slattery, 1967 and 1969; Gray and O'Neill, 1976; Whitaker, 1986a). Consequently, it is easy to extend to non-Darcy flow and multiphase flow (see Section 2.4).
2.3 Miscible Displacement

2.3.1 Mathematical model

For studying enhanced recovery projects, an important simplification of the fully compositional model is the case where the components mix together and form a single phase. This is called miscible displacement. In addition to reservoir simulation, there are applications to groundwater pollution modeling, such as the transport of salt, polymers or contaminants in water. The simplest model problem for miscible displacement is the one-dimensional convection-diffusion equation:

\[
\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = D \frac{\partial^2 C}{\partial x^2}.
\]  

(2.37)

Its assumptions are that there are two components which mix together to form a single phase that is incompressible. In one dimension, the velocity, \( u \), and diffusion coefficient, \( D \), may be assumed constant. For suitable boundary conditions, this equation has a known solution in terms of the error function which is frequently used as a test of numerical methods.

While it is relatively easy to solve the one-dimensional problem, the real test of a numerical method comes in applying it in two dimensions. Then, both the pressure and concentration must be solved for. A favorite geometry for test purposes is the repeated five-spot pattern, which is an infinite array of injection and production wells. (See Figure 2.7). Each injector is surrounded by four producers, and each producer by four injectors. The basic symmetry element is the triangle. However, square symmetry elements are usually used in test calculations, in order to simplify the programming.

There are two ways of orienting a grid, the diagonal grid, and the parallel grid. In the diagonal grid, the main flow path between the injection and production well is diagonal to the grid. In the parallel grid, the main flow path is parallel to the grid lines. The same answers should, of course, be obtained with either grid. But, very different answers can be obtained, due to preferential flow along the grid lines. This is known as the grid orientation effect (Coat et al., 1974). Considerable research is being devoted to devising numerical methods to reduce this grid orientation effect (Yanosik and McCracken, 1978; Shubin and Bell, 1984).

The two-dimensional analogue of Equation (2.37) cannot assume constant velocity,
so the convection-diffusion equation is coupled to an elliptic equation that determines pressure and, by Darcy's law, velocity. In a horizontal plane domain, we write the equation set as

\[ u = -\frac{k}{\mu(\varepsilon)} \nabla p, \]  
(2.38)

\[ \nabla \cdot u = q, \]  
(2.39)

\[ \frac{\partial (\phi C)}{\partial t} + \nabla \cdot (C u) - \nabla \cdot (\phi D \nabla C) = \hat{C} q. \]  
(2.40)

With no-flow boundary conditions

\[ u \cdot n = \nabla C \cdot n = 0 \]  
(2.41)

and the initial concentration

\[ C = C_0. \]  
(2.42)
The dependent variables are pressure $p(x, t)$ and solvent concentration $C(x, t)$, $0 \leq C \leq 1$. The source/sink term $q(x, t)$ is the volumetric flow rate per unit volume at the wells. Since a well is very small compared to the domain, $q$ is nearly a combination of singular Dirac measures. The porosity $\phi(x)$ is the fraction of total volume available for porous flow. By $\hat{C}(x, t)$ we represent injected concentration at sources (injection wells) and resident concentration at sinks (production wells). The dispersion tensor $D(x, \nu)$ is discussed in the next paragraph. Physically, Equation (2.38) is Darcy's law, and Equations (2.39) and (2.40) represent conservation of mass for the fluid mixture and the solvent, respectively. If combined, Equations (2.38) and (2.39) form an elliptic equation known as the pressure equation. We call Equation (2.40) the concentration equation, which is a dispersion-diffusion equation. Note that Equation (2.40) depends on $p$ through $u$, and that the pressure equation depends on $C$ through $\mu$. We assume the quarter power viscosity law $\mu(C)^{-\frac{1}{4}} = (1 - C)\mu(0)^{-\frac{1}{4}} + C\mu(1)^{-\frac{1}{4}}$ and define the mobility ratio $M = \frac{\mu(0)}{\mu(1)}$. For $M > 1$, or adverse mobility ratio, the solvent is less viscous than the oil, and experiments predict that the displacement front will be physically unstable, so that the solvent will form fingers into the oil.

The dispersion tensor is given by

$$D = D_m + \frac{\alpha_t}{|u|} \begin{pmatrix} u_x^2 & u_x u_y \\ u_x u_y & u_y^2 \end{pmatrix} + \frac{\alpha_t}{|u|} \begin{pmatrix} u_y^2 & -u_y u_x \\ -u_y u_x & u_x^2 \end{pmatrix},$$

(2.43)

where $D_m$ is the molecular diffusivity (units: $\text{length}^2/\text{time}$), and $\alpha_l$ and $\alpha_t$ are the longitudinal and transverse dispersivities (units: $\text{length}$), respectively. In practical problems, $D_m$ is small compared to the other terms and will be neglected. If $L$ is a characteristic length of the displacement, such as the distance from an injection well to a production well, the longitudinal and transverse Peclet numbers (ratios of convection to dispersion) are defined by

$$Pe_l = \frac{L}{\alpha_l} \quad \text{and} \quad Pe_t = \frac{L}{\alpha_t}.$$ 

(2.44)

The appropriate range for $Pe$ in field problems is in the tens or hundreds. In this study we use a diagonal dispersion tensor in which the cross-derivative terms of Equation (2.43) are neglected. The absence of these cross-derivative terms is only for simulations on a square lattice, not essential for simulations on a hexagonal lattice. A similar
situation exists with the industry’s most popular method, the five-point difference operator.

2.3.2 Lattice Boltzmann methods

Pure diffusion or reaction-diffusion equations have recently been approximated using the lattice gas and the lattice Boltzmann techniques (i.e., Ponce Dawson et al., 1992). These methods are able to reproduce the fundamental physical phenomena seen in diffusion systems, such as chemical waves and the Turing instability, and provide a parallel computing algorithm for solving these equations. The major advantage of the lattice gas and lattice Boltzmann method over traditional numerical techniques, such as finite difference schemes, is that they provide insight into the underlying microscopic dynamics of the physical system investigated, whereas most methods focus only on the solution of the macroscopic equations. On the other hand, the lattice gas and lattice Boltzmann methods are much faster than full molecular dynamics simulations, because they involve some degree of averaging. In particular, the lattice Boltzmann method provides a computationally efficient approach due to its intrinsic parallelism. These models might be useful to study the convection-diffusion phenomena in porous media and to determine the so-called dispersion tensor (Salles et al., 1993). However, we will introduce a new lattice Boltzmann method for directly solving the dispersion-diffusion equations (2.40) plus the fluid mixture described by Darcy’s law (2.38). In Section 2.2 we have discussed the lattice Boltzmann model for single phase Darcy flow in porous media which could be used to simulate the evolution of the fluid mixture for the miscible fluid. This section will be devoted to the lattice Boltzmann model for simulating the dispersion-diffusion equations.

Following Section 2.2, the lattice Boltzmann equation for the one-particle distribution function of species \( i \) can be written as

\[
 f_i(x + e_i, t + 1) - f_i(x, t) = \Omega_i(x, t),
\]

where \( \Omega \) is the collision operator for the species that depends on the distribution function \( f(x, t) \). All the quantities in this equation are dimensionless. In particular, time is measured in units of the time step \( \Delta t \) and space in units of the mesh size \( \Delta x \).
Thus $x$ and $t$ are related to the spatial and time coordinates of the original Equation (2.40) by $X_j = x_j \Delta x_j$ and $T = t \Delta t$.

In order to relate the result obtained by solving Equation (2.45) with the solution of Equation (2.40), we derive the evolution equations for the moments of the function, $f^s$. Let us consider a two-dimensional case with $\Delta x = \Delta x(\hat{x} + \hat{y})$. Then, the zeroth moment of $f^s$, the local densities of species at time $t$ and position $x$, defined by

$$\rho_s(x, t) = \sum_i f^s_i(x, t),$$

(2.46)
can be related to the concentration $C$ of Equation (2.40) by $\rho_s = C \phi \gamma^s$, where $\gamma^s$ is the true density of species. As before, for $\Omega^s_i$, we use the single relaxation time or BGK approximation,

$$\Omega^s_i(x, t) = -\frac{f^s_i(x, t) - f^s_{eq}(x, t)}{\tau^s_i},$$

(2.47)

where the equilibrium distribution function, $f^s_{eq}$, depends on $x$ and $t$ through the local density and velocity. Note that here the relaxation time, $\tau^s$, depends on the direction. For convenience, we assume that $\tau^s_0 = \tau^s_1 = \tau^s_x$ and $\tau^s_1 = \tau^s_y = \tau^s$. As in the usual Chapman-Enskog expansion, we impose the following conditions on $f^s_{eq}$:

$$\sum_i f^s_i(x, t) = \sum_i f^s_{eq}(x, t) = \rho_s(x, t),$$

(2.48)

$$\sum_i e_i f^s_{eq}(x, t) = \rho_s(x, t) v_s(x, t),$$

(2.49)

where $v_s(x, t)$ is the local velocity of species. Equation (2.49) represents the conservation of local mass for a nonreactive system. To obtain solutions of Equation (2.40), we use the following local velocity of the species,

$$v_s(x, t) = v(x, t) + \frac{\Pi^s(x) \cdot \nabla \phi(x)}{\rho_s(x, t) \phi(x)},$$

(2.50)

where $\Pi^s = \begin{pmatrix} \tau^s_x & 0 \\ 0 & \tau^s_y \end{pmatrix}$ and $v(x, t)$ is the fluid mixture velocity, defined in Section 2.2.

To derive the evolution equation for concentration $C$ from Equation (2.45), we expand $f^s_i(x + e_i, t + 1)$ in a Taylor series around $f^s_i(x, t)$, obtaining,

$$f^s_i(x + e_i, t + 1) - f^s_i(x, t) = \sum_{n=0}^{\infty} \frac{1}{n!} \left[ \frac{\partial}{\partial t} + (e_i \cdot \nabla) \right]^n f^s_i(x, t) = \Omega_i,$$

(2.51)
We then expand $f_i^s$ around the equilibrium distribution as $f_i^s \approx f_i^{s(eq)} + f_i^{s(1)}$ and assume the scaling: $f_i^{s(1)} \sim \epsilon$. The following multiscaling is also assumed: $\partial / \partial t \sim \epsilon^2$, $\partial / \partial x \sim \epsilon$, where $\epsilon$ is a small parameter. Then, Equation (2.51) can be separated into two parts,

$$(e_i \cdot \nabla) f_i^{s(eq)}(x, t) = -\frac{f_i^{s(1)}(x, t)}{\tau_i^s}$$  \hspace{1cm} (2.52)

and

$$\frac{\partial f_i^{s(eq)}(x, t)}{\partial t} + (e_i \cdot \nabla) f_i^{s(1)}(x, t) + \frac{1}{2}(e_i \cdot \nabla)^2 f_i^{s(eq)}(x, t) = O(\epsilon^3).$$  \hspace{1cm} (2.53)

From Equation (2.52), we obtain

$$f_i^{s(1)}(x, t) = -\tau_i^s (e_i \cdot \nabla) f_i^{s(eq)}(x, t).$$  \hspace{1cm} (2.54)

Substituting Equation (2.54) into Equation (2.53) leads to

$$\frac{\partial f_i^{s(eq)}(x, t)}{\partial t} - (e_i \cdot \nabla) [\tau_i^s (e_i \cdot \nabla) f_i^{s(eq)}(x, t)] + \frac{1}{2}(e_i \cdot \nabla)^2 f_i^{s(eq)}(x, t) = O(\epsilon^3).$$  \hspace{1cm} (2.55)

Adding Equations (2.52) and (2.55) and doing some simple algebra, we have to order $\epsilon^2$,

$$\frac{\partial \rho_s}{\partial t} + \nabla \cdot (\rho_s v_s) - \frac{1}{2} \nabla \cdot [\Pi^s - \frac{1}{2} I] \cdot \nabla \rho_s = 0,$$  \hspace{1cm} (2.56)

for the density of the species, or

$$\frac{\partial C}{\partial t} + \nabla \cdot (C u) - \frac{1}{2} \nabla \cdot [\phi (\Pi^s - \frac{1}{2} I) \cdot \nabla C] = 0,$$  \hspace{1cm} (2.57)

for the concentration of the species, where $I$ is the unit tensor.

Comparing Equation (2.57) with the original dispersion-diffusion equation (2.40), we obtain the relation between the dispersion tensor in the real system and relaxation parameter tensor $\Pi^s$ in the lattice Boltzmann system, namely, $D = \frac{1}{2} (\Pi^s - \frac{1}{2} I)$.

As with other finite difference schemes, the accuracy of the solution obtained from the lattice Boltzmann method depends on the choice of the space and time discretization. In order to demonstrate how to apply the lattice Boltzmann method for simulation of miscible displacement in porous media described by the dispersion-diffusion equation and the accuracy of lattice Boltzmann simulation of physical problems we present three typical numerical examples.
Figure 2.3: Solutions of the 1-D convection-diffusion equation at different injected pore volumes.

2.3.3 Numerical simulations

The lattice Boltzmann scheme proposed here has been applied to the 1-D convection-diffusion equation and to 2-D miscible flooding problems. The 1-D computations were conducted to verify the validity of the numerical scheme by comparison with analytical solutions. The 2-D problems demonstrate applicability of the scheme to large-scale reservoir simulations.

The exact solution to the convection-diffusion equation (2.37) for a semi-infinite system is (i.e., Bear, 1972)

$$C(x,t) = \frac{1}{2} \text{erfc} \left( \frac{x - vt}{\sqrt{2Dt}} \right) + \frac{1}{2} \exp \frac{vx}{D} \text{erfc} \left( \frac{x + vt}{\sqrt{2Dt}} \right).$$  \hspace{1cm} (2.58)

This solution satisfies the initial condition $C(x,0) = 0$ and the boundary conditions $C(0,t) = 1$ and $\lim_{x \to \infty} C(x,t) = 0$. Accordingly, this solution is only comparable to the numerical solution of a finite length before breakthrough. Typically, the most difficult situation to handle numerically is the convection-dominated flow (Stone and Brian, 1963). This is very distressing because most EOR processes are associated with sharp displacement fronts, which are characteristic of convection-dominated problems.
To test the lattice Boltzmann method for this case, the model problem to be solved has a Peclet number of 1000. Sixty five gridblocks are used, which results in a cell Peclet number of 15. Figure 2.8 shows the concentration profiles obtained with the lattice Boltzmann method at several times. The analytical solutions have been superimposed for comparison. Good agreement with the analytical solution is observed.

In the next numerical example we will describe applications of the proposed lattice Boltzmann method to 2-D miscible displacement in porous media. All the numerical results are computed on a repeated five-spot pattern with $M=41$, $Fe=100$, constant porosity, and uniform or random permeabilities. As noted in previous sections, the uniform-permeability case is not physically relevant and cannot be attained in practice. However, we (more or less) know what its solution should look like, and this makes it useful in the evaluation of numerical methods. To examine grid orientation, a quarter of the pattern was modeled with a diagonal grid of mesh size 50 X 50, and a parallel grid of mesh size of 71 X 71. In the plots that follow, the injector is at the lower-left corner and the producer at the upper-right (the parallel grid is just rotated 45 degrees). Figures 2.9 and 2.10 show the contour plots of concentration at 0.4 and 0.6 pore volume injected (PVI), shortly before and after solvent breakthrough at the production well for the problems considered, respectively. Experience has shown that the worst anomalies in the solution will appear around this time; if the solution is good near breakthrough, it should be good at other times. As Figures 2.9 and 2.10 make clear there is no significant grid orientation sensitivity. The recovery curves plotted on Figure 2.11 indicate that overall differences between diagonal and parallel grids are less than 5%, which is much better than results from finite difference methods (Settari et al., 1977).

Next, we consider variations in the mesh size. Figure 2.12(a) uses 100 X 100 grids, Figure 2.12(b) uses 50 X 50 grids, and Figure 2.12(c) uses 25 X 25 grids. Figure 2.13 shows the recovery curves for these runs with the 100 X 100, 50 X 50 and 25 X 25 grids of Figure 2.12. We see very little difference between Figures 2.12(a), 2.12(b), and 2.12(c) or between their associated recovery curves in Figure 2.13. The curves appear to be converging at a first-order rate, or maybe a bit better than that. The 25 X 25 front is somewhat dispersed because the mesh is too coarse to resolve it. Note that the interval in this case is only about half of the front width in Figure 2.12(a).
Figure 2.9: Concentration contours of diagonal (50 X 50) and parallel (71 X 71) grids at 0.4 PVI, just before solvent breakthrough at production wells.
Figure 2.10: Concentration contours of (a) diagonal (50 X 50) and (b) parallel (71 X 71) grids at 0.6 PVI, just after solvent breakthrough at production wells.
Figure 2.11: Recovery curves for diagonal (50 X 50) and parallel (71 X 71) grids.

That means that in this mesh there are only two intervals across the front, and this is not quite enough. These results indicate that there is no significant mesh-dependent numerical dispersion as long as a front is resolved by about 3 intervals.

Finally, we give some examples with varying permeability, as opposed to the physically irrelevant constant permeability used to this point. It has long been observed that the adverse-mobility-ratio displacement fronts are physically unstable; small perturbations of a smooth front grow into multiple viscous fingers. (By adverse mobility, we mean that the viscosity of the injected fluid is less than that of the resident fluid). The previous results give us confidence that any fingering produced in a heterogeneous analogue of the base case will be physical, not numerical. To define the permeability heterogeneity, it is usual to characterize two parameters: permeability variance and scale length. The permeability variance characterizes the extent of heterogeneity, whereas the scale length characterizes the size of heterogeneity. In this study, the permeability distribution was assumed to be log-normal. For the log-normal distribution, the permeability variance can be defined by the Dykstra-Parsons coefficient (Dykstra and Parsons, 1950). The Dykstra-Parsons coefficient, $v$, is related to $\sigma$, the standard deviation of the log-normal permeability distribution, by $\sigma = \ln[1/(1 - v)]$. The
[Figure is concluded on the next page.]
Figure 2.12: Concentration contours of 100 X 100 (a), 50 X 50 (b) and 25 X 25 (c) diagonal grids at 0.6 PVI.

scale length of the distribution is estimated by calculating the length over which the neighboring permeability values are related to each other. As this distance increases, so does the scale-length value. Typically, scale length is quantified by plotting an autocovariance function on the y axis vs. a lag distance on the x axis for a 2-D problem. The point where the autocovariance function intercepts the x axis is the measure of scale length. Another measure of permeability heterogeneity that combines the scale length and the permeability variance is the heterogeneity index, \( I_H \), defined as \( I_H = \sigma^2 L_{SD} \), where \( L_{SD} \) is the dimensionless scale length: i.e., ratio of scale length to the system length. In this study, we use a relatively small values of heterogeneity index (\( I_H < 0.2 \)). Figures 2.14(a) and 2.14(b) show the concentration contours at \( I_H = 0.2 \) and \( I_H = 0.1 \), respectively. Both plots are qualitatively similar to the laboratory displacement cited by Peaceman (Peaceman, 1986) and the numerical simulation obtained by high-order, finite difference flux-corrected transport (FCT) methods (Christie, 1989). Figures 2.14(a) and 2.14(b) also show that the higher the
variation is, the greater the concentration fluctuations. This means that an increase in permeability variance increases the instability.

Next we consider the experiment of Blackwell et al. (1959). Several investigators (Peaceman and Rachford, 1962; Christie and Bond, 1987; Hatzivramidis, 1990) have matched their experimental recovery profiles. Simulation data for mobility ratios of 5 and 86 were generated for comparison with these experiments using a grid of 80 X 240. Figure 2.15 shows the growth of viscous fingers for M=5 case after 0.2, 0.4, and 0.6 PVI. As in Peaceman and Rachford's (1962) work, multiple small fingers present are at the time after 0.2 PV injected and at later times these fingers collapse into one dominant finger that continue to exist at times after breakthrough. The oil recovery for the mobilities of 5 and 86 as a function of solvent injected is shown in Figure 2.16. The good agreement between numerical simulation obtained and experimental data
Figure 2.14: Concentration contours of 100 X 100 diagonal grids with $I_H = 0.2$ (a) and $I_H = 0.1$ (b), at 0.6 PVI.
Figure 2.15: Finger evolutions for $M=5$ at 0.2, 0.4, and 0.6 PVI.
Figure 2.16: Comparison of experimental and simulated recoveries for \( M=5 \) and \( M=86 \) (Blackwell et al., 1959).

is encouraging, though for the mobility ratio of 86, the breakthroughs do not match. However, the later experimental values are reasonably close to the numerical values.

2.3.4 Concluding remarks

A numerical method was developed for the simulations of miscible displacement processes. This method can be extended to 3-D and reactive dispersion-diffusion equations with several species. By comparing results obtained from this method with analytical solutions for the 1-D convection-diffusion equation, the method was shown to resolve sharp displacement fronts in convection-dominated flows. The method was also shown to be convergent and insensitive to grid orientations. The method was also shown to be capturing the instabilities to perturbation in 2-D displacements with unfavorable mobility ratios. In particular, computations of displacements with highly unfavorable mobility ratios showed that these displacements remain stable in the absence of perturbations; the same displacements are shown to become unstable when perturbations of minute size are introduced. The perturbations required to render un-
stable displacements with unfavorable mobility ratios were introduced in the form of permeability variations. Computations of unstable displacements showed a finger evolution similar to that determined experimentally.

2.4 Immiscible Multiphase Flow

2.4.1 Mathematical formulation

In last section, we have discussed the case where two fluids are completely soluble in each other. The interfacial tension between the two fluids is zero, and the two fluids dissolve in each other. A distinct fluid-fluid interface does not exist. In this section we will discuss the case where there is a simultaneous flow of two immiscible fluids or phases (e.g., oil, water and gas) in the porous medium. The interfacial tension between the two fluids is nonzero, and a distinct fluid-fluid interface separates the fluids within each pore. A capillary pressure difference exists across the interface at each point on it.

Although this immiscible displacement process occurs at microscopic level, however, continuum models are usually used in reservoir engineering. Many investigators conclude from experiments that when two immiscible fluids flow simultaneously through a porous medium each fluid establishes its own tortuous path, which forms very stable channels. They assume that a unique set of channels corresponds to every degree of saturation (S). If a wetting fluid (at $S_w$) and a nonwetting fluid (at $S_o$) are being considered, as $S_o$ is reduced, the channels of the nonwetting fluid tend to break down until only isolated regions of it remain at residual nonwetting fluid saturation. Similarly, as $S_w$ decreases, the channels of wetting fluid tend to break down and become discontinuous at the irreducible wetting fluid saturation. When any of these fluids become discontinuous throughout the flow domain, no flow of that fluid can take place. With these concepts in mind, it seems natural to apply the concept of permeability established for the flow of a single-phase fluid through a porous medium, modifying its value owing to the presence of the second phase. It is common to generalize Darcy’s law by applying it to the two phases separately and simultaneously at each location.
i.e. setting at each point

\[ u_I = -\frac{k_I}{\mu_I} \cdot (\nabla p_I - \gamma g \nabla h), \]  

(2.59)

where \( u_I \) is the phase velocity. \( k_I \) is the phase permeability, \( \mu_I \) is the phase viscosity. \( p_I \) is the phase pressure. and \( \gamma g \nabla h \) is the gravity term. The wetting fluid and nonwetting fluid pressures, \( p_w \) and \( p_o \), are often taken to differ by a macroscopic pressure difference

\[ p_c = p_o - p_w, \]  

(2.60)

which must have the magnitude of the surface tension divided by a pore diameter. i.e... about half an atmosphere. This capillary pressure and separate permeabilities to the wetting fluid and nonwetting fluid. \( k_w \) and \( k_o \), that are allowed depend on the oil saturation. \( S_o \). Note that

\[ S_w + S_o = 1. \]  

(2.61)

The two permeabilities are routinely measured in laboratories by pumping a mixture of them through a sample of rock. Quite small samples may be obtained in a reasonable time, bearing in mind the very slow rates appropriate to reservoir conditions (cms/day). The measured permeabilities are expressed as a fraction of the value that they have when there is only the one phase present. this fraction being known as the relative permeability, defined as

\[ k_{r,I} = \frac{k_I}{k}. \]  

(2.62)

where \( k \) is the permeability of the medium to a single-phase fluid completely saturating it. and sometimes is called intrinsic permeability.

It should be pointed out that although this generalization to multiphase flow is very natural and is universally employed, it has no theoretical justification, such as the derivation of the law for single-phase flow. and invokes several implicit assumptions. A fundamental assumption is that flow of the respective phase is not directly affected by pressure gradients in another phase. This, it may be noted, is not absolutely true but requires that slippage zones at phase interfaces are thin relative to the total film thicknesses of the phases. The assumption may be increasingly prone to break down in fine-grained porous media and at low fluid saturations: however, since separate permeabilities, \( k_w \) and \( k_o \), will become extremely low under such circumstances. this difficulty probably is moot from a practical point of view. There have been suggestions
that cross flow drag terms should also be included in the equation of motion (de la Cruz and Spanos, 1983. Whitaker, 1986b). Another critical assumption is the validity of the concept of intrinsic permeability which purports to separate fluid-dependent and porous medium-dependent effect on fluid flow. The assumption that intrinsic permeability is a unique (tensorial) characteristic of the porous medium is again prone to break down for fine-grained materials. as such material can in fact exhibit order of magnitude differences in “intrinsic” permeability when saturated with different fluids. Furthermore, the notion that the tensorial nature of fluid conduction can be relegated to a tensor while relative permeability remains a scalar has little to justify itself beyond convenience. Recent evidence in fact indicates that relative permeability may have a tensorial nature that varies with fluid saturation (Bear et al., 1987). This is unfortunate because it adds considerable complication to an already difficult problem.

The conservation of mass for each phase is expressed by the relation

$$\frac{\partial (\varphi \gamma_i S_i)}{\partial t} = -\nabla \cdot (\gamma_i u_i) + q_i. \quad (2.63)$$

where $\varphi$ is the medium porosity, $S_i$ is the fraction of the pore space containing phase $i$ (phase saturation), $\gamma_i$ is the phase density, $u_i$ is the Darcy velocity of phase $i$, and $q_i$ is the phase mass injection or production rates (source or sink terms) which are used to model wells. Substituting Darcy’s equation of $u_i$ yields

$$\frac{\partial (\varphi \gamma_i S_i)}{\partial t} = \nabla \cdot \frac{\gamma_i \kappa_i}{\mu_i} (\nabla p_i - \gamma_i g \nabla z) + q_i. \quad (2.64)$$

The system of Equation (2.64) is coupled by constraints of Equations (2.60) and (2.61). The phase densities are also functions of phase pressures and are obtained from an equation of state. For a slightly compressible liquid it is convenient to write.

$$c_i = \frac{1}{\gamma_i \frac{\partial \gamma_i}{\partial p_i}}|_T. \quad (2.65)$$

where $c_i$ is the phase compressibility at constant temperature, $T$. Separating the variables in Equation (2.65) and denoting $\gamma_{ib}$ as the phase density at pressure $p_{ib}$, we obtain.

$$\gamma_i = \gamma_{ib} \exp[c_i(p_i - p_{ib})]. \quad (2.66)$$

If the compressibility, $c_i$, is small (as it usually is for the oil and water phases), a further simplification is possible. A truncated Taylor series expansion for the exponential term
in Equation (2.66) yields,
\[ \gamma_t = \gamma_b [1 + c_t (p_t - p_b)]. \] (2.67)

It is important to recognize the nature of the highly non-linear Equation (2.64). To demonstrate this consider the classical Buckley-Leverett problem of one-dimensional, two-phase, incompressible flow of oil and water with no gravity effects. This solution has frequently been used as a comparison with which to test many reservoir simulations. The Equation (2.64) becomes
\[ \phi \frac{\partial S_o}{\partial t} = \frac{\partial}{\partial x} \left( \lambda_o \frac{\partial p_o}{\partial x} \right), \] (2.68)
\[ \phi \frac{\partial S_w}{\partial t} = \frac{\partial}{\partial x} \left( \lambda_w \frac{\partial p_w}{\partial x} \right) \] (2.69)

where the phase mobility, \( \lambda_t \), is defined as,
\[ \lambda_t = \frac{k k_{rt}}{\mu_t}. \] (2.70)

Adding Equations (2.68) and (2.69), with \( \partial S_o/\partial t = -\partial S_w/\partial t \) from Equation (2.61), gives,
\[ \frac{\partial}{\partial x} \left( \lambda_o \frac{\partial p_o}{\partial x} \right) + \frac{\partial}{\partial x} \left( \lambda_w \frac{\partial p_w}{\partial x} \right) = 0. \] (2.71)

Substituting Equations (2.60) gives,
\[ \frac{\partial}{\partial x} \left( \lambda_T \frac{\partial p_o}{\partial x} \right) - \frac{\partial}{\partial x} \left( \lambda_w \frac{\partial p_c}{\partial x} \right) = 0, \] (2.72)

where the total mobility is defined as, \( \lambda_T = \lambda_o + \lambda_w \). Equation (2.72) is usually referred to as the pressure equation. Next, we define the water fractional flow, \( f_w \), as
\[ f_w(S_w) = \frac{\lambda_w}{\lambda_o + \lambda_w} = \frac{\lambda_w}{\lambda_T}. \] (2.73)

Utilising Equation (2.70), Darcy’s law may now be written as,
\[ u_o = -\lambda_o \frac{\partial p_o}{\partial x}, \quad \text{and} \quad u_w = -\lambda_w \frac{\partial p_w}{\partial x}, \] (2.74)

which together with Equation (2.60), may be used to expand the RHS in Equation (2.69) as,
\[ \frac{\partial}{\partial x} \left( \lambda_w \frac{\partial p_w}{\partial x} \right) = -\frac{\partial}{\partial x} (f_w u_T) - \frac{\partial}{\partial x} \left( f_w \lambda_o \frac{\partial p_c}{\partial x} \right), \] (2.75)
Figure 2.17: Fractional flow function for the immiscible, two-phase problem.

where the total velocity is defined as, \( u_T = u_o + u_w \). Substitution of Equation (2.75) into Equation (2.69), with the observation that for incompressible flow \( u_T \) is a constant, yields

\[
\phi \left( \frac{\partial S_w}{\partial t} \right) + u_T \left( \frac{\partial f_w}{\partial x} \right) + \frac{\partial}{\partial x} \left( f_w \lambda_o \frac{\partial p_C}{\partial x} \right) = 0,
\]

(2.76)

Equation (2.76) is known as the total velocity form of the saturation equation. We note that Equation (2.72), the pressure equation, and Equation (2.76), the saturation equation, are alternative forms for the system conservation Equations (2.68) and (2.69).

For the classical Buckley-Leverett problem, with zero capillary pressure, Equation (2.76) reduces to,

\[
\frac{\partial S_w}{\partial t} + \frac{\partial f_w}{\partial x} = 0,
\]

(2.77)

where we have set \( u_T/\phi = 1 \) without loss of generality.

Equation (2.77) is known to have multiple weak solutions displaying shocks or discontinuities (Lax, 1972). It has been shown that the physically relevant solution may be identified as a limit of solutions to the equation (Taggart and Pinczewski, 1987)

\[
\frac{\partial S_w}{\partial t} + \frac{\partial f_w}{\partial x} = \epsilon \frac{\partial^2 S_w}{\partial x^2},
\]

(2.78)
as ε-dissipation approaches zero. The discontinuities of such solutions satisfy the entropy condition (Glimm, 1988)

$$\frac{f(S_w) - f(S_{w,L})}{S_w - S_{w,L}} \geq s \geq \frac{f(S_w) - f(S_{w,R})}{S_w - S_{w,R}}$$

(2.79)

for all $S_w$ between $S_{w,L}$ and $S_{w,R}$, where $S_{w,L}$ and $S_{w,R}$ are the states on the left and on the right of the discontinuity, respectively. The speed of propagation of the discontinuity, $s$, is given by the Rankin–Hugoniot relation,

$$f(S_{w,R}) - f(S_{w,L}) = s(S_{w,R} - S_{w,L}).$$

(2.80)

It is easy to show by a geometric construction of Equations (2.79) and (2.80) that all initial state pairs, $S_{w,L}$ and $S_{w,R}$, satisfy the entropy condition if the flux function, $f_w$, is purely convex or concave. Unfortunately, this is not the case for the type of flow considered here. For two-phase flows in a porous medium the relative permeabilities are typically quadratic in each of the phase saturations. This leads to the following expressions for water fractional flow and its first derivative as functions of water saturation (Taggart and Pinczewski, 1987),

$$f_w = \frac{S_w^2}{S_w^2 + \frac{\mu_w}{\mu_w} (1 - S_w)^2},$$

(2.81)

and

$$\frac{df_w}{dS_w} = \frac{2 \frac{\mu_w}{\mu_w} S_w (1 - S_w)}{\left[ S_w^2 + \frac{\mu_w}{\mu_w} (1 - S_w)^2 \right]^2}.$$  

(2.82)

The form of these functions for the case $\frac{\mu_w}{\mu_w} = 1$ is shown in Figure 2.17. The flux function is clearly not purely convex or concave for all $S_w$, but has a point of inflection. The non-convexity of the flux function implies that in the close vicinity of the inflection point it is not possible to satisfy the entropy condition. This means that all numerical schemes which have order of accuracy greater than one (i.e. all higher-order schemes) will produce solutions which contain entropy violating shocks and which, therefore, are not physically relevant. There is, as yet, no satisfactory solution for this problem and all practical numerical schemes which have accuracy greater than one require some sort of flux correction (e.g., addition of artificial dissipation) in the vicinity of inflection points to ensure convergence to a physical relevant solution.
2.4.2 Numerical methods

We adopt a numerical scheme appropriate to two-dimensional reservoir simulation that is based on the Boltzmann transport equation with computations performed at the intersections of a rectangular grid or lattice. The most common application of the lattice Boltzmann method has been to fluid flow models for which mass and momentum are conserved. Applications of the lattice Boltzmann method to multiphase flows in porous media are limited to microscopic levels, where Navier-Stokes equation instead of Darcy’s law are employed. As we have stated earlier, the continuum approach of multiphase fluid flow is just a generalization of Darcy’s law of single phase in porous media. So too is our lattice Boltzmann model. In the following we will generalize the lattice Boltzmann model in Section 2.2 for single phase flow to multiphase fluid flow in a porous medium. For simplicity we restrict our consideration to an incompressible, two-phase, immiscible, two-dimensional fluid model. Computer code based on these considerations results in an effective waterflood simulator.

The starting point of the lattice Boltzmann method is the kinetic equation for the velocity distribution function. Let \( f_i^w(x, t) \) and \( f_i^n(x, t) \) be the mass densities of the wetting (w) and nonwetting (n) fluids, respectively, at site \( x \) and time \( t \) moving along a link in the \( i \) direction. Here \( i = 1, 2, \cdots, N \), where \( N \) is the number of allowable velocity states at each site. The kinetic or “lattice-Boltzmann” equation for \( f_i \) of phase \( l \) is written

\[
f_i^l(x + e_i, t + 1) - f_i^l(x, t) = \Omega_i^{l(c)} + \Omega_i^{l(d)},
\]

(2.83)

where \( \Omega_i^{l(c)} \) is the term representing the rate of change of \( f_i^l \) due to collisions, and \( \Omega_i^{l(d)} \) is the term representing flow damping in a porous medium. The vectors \( e_i \) are the velocity vectors along the links of the lattice.

For computational efficiency, we have used a square lattice (\( N = 4 \)) and the single time relaxation model (Qian et al, 1992) with the linear collision operator:

\[
\Omega_i^{l(c)} = \frac{1}{\tau^l}(f_i^l - f_i^{l(eq)}),
\]

(2.84)

where \( \tau^l \) is the characteristic relaxation time, and \( f_i^{l(eq)} \) is the local equilibrium distribution given by

\[
f_i^{l(eq)} = \frac{\rho_i}{4}(1 + 2e_i \cdot v_i).
\]

(2.85)
In the above equations \( \rho_l = \sum f_i^l \) and \( \rho_l v_i = \sum f_i^l e_i \) are the local phase bulk density and momentum, respectively.

Defining the damping resistance by \( F_l \), we add the momentum damping term

\[
\Omega_i^{l(d)} = \frac{1}{2} F_l \cdot e_i,
\]  

(2.86)

to facilitate the momentum dissipation of flow through the porous medium. The detailed forms of the resistance \( F_l \) will be determined by the hydrodynamical equations of fluid flow through porous media.

To derive hydrodynamics, take the long-wavelength, low-frequency limit of Equation (2.83), to obtain

\[
\frac{\partial f_i^l}{\partial t} + e_i \cdot \nabla f_i^l + \frac{1}{2} e_i e_i : \nabla \nabla f_i^l = \Omega_i^{l(c)} + \Omega_i^{l(d)}.
\]  

(2.87)

Using definitions (2.84) and (2.86) for collision and damping operators, Equation (2.87) leads, after summation, to the mass conservation,

\[
\frac{\partial \rho_l}{\partial t} + \nabla \cdot (\rho_l v_l) = 0,
\]  

(2.88)

and, after multiplication with \( e_i \), summation and deletion of second, and higher, order terms, leads to the following momentum equation,

\[
\frac{\partial \rho_l v_l}{\partial t} = -\frac{1}{2} \nabla \rho_l + F_l.
\]  

(2.89)

For a slow flow like Darcy flow in porous media the convective terms are generally negligible. Thus, Equation (2.89) reduces to

\[
\nabla \sigma_l = F_l.
\]  

(2.90)

where \( \sigma_l = \frac{1}{2} \rho_l \) is the local bulk pressure. Note that this is the equation of state for an isothermal ideal gas. However, one may come arbitrarily close to solving incompressible flows by reducing the Mach number. This approach has much in common with explicit “penalty” or “pseudocompressibility” methods of solving incompressible flows. Since the traditional hydrodynamical equations in porous media are usually given in terms of the true fluid density (\( \gamma_l \)), pore pressure (\( p_l \)) and Darcy (bulk) velocity (\( u_i^l \)), defined as

\[
\gamma_l = \frac{\rho_l}{\partial S_l}, \quad p_l = \frac{\sigma_l}{\partial S_l}, \quad \text{and} \quad u_i^l = \phi S_l v_i,
\]  

(2.91)

66
the final mass and momentum become

\[ \frac{\partial (\phi S_l \gamma_l)}{\partial t} + \nabla \cdot (\gamma_l u_l) = 0, \]  
\[ \frac{\nabla \phi}{\phi} + \frac{\nabla S_l}{S_l} + \frac{\nabla \gamma_l}{\gamma_l} = \frac{2F_l}{\phi S_l \gamma_l}. \]  
\[ (2.92) \]
\[ (2.93) \]

To solve for \( F_l \), substitute Equations (2.59)–(2.61) into Equation (2.93) and note that

\[ \gamma_l u_l = \rho_l v_l + \frac{F_l}{2}, \]  
\[ (2.94) \]

where \( \rho_l v_l \) and \( \rho_l v_l + F_l \) are the local momentum before and after collisions, respectively. We have the final expression for the momentum proportional resistances,

\[ F_w = \frac{[(c_w(\lambda_w^\gamma + a_o) + b_w(c_w^\gamma \lambda_w^\gamma)\lambda_w^\gamma \nabla \phi}{\lambda_w^\gamma]} - 2a_w(\lambda_w^\gamma + a_o)\rho_w v_w - 2a_o b_w \lambda_w^\gamma \rho_o v_o, \]
\[ F_o = \frac{[(c_o(\lambda_w^\gamma + a_w) + b_o(c_o^\gamma \lambda_w^\gamma)\lambda_o^\gamma \nabla \phi}{\lambda_o^\gamma]} - 2a_o(\lambda_w^\gamma + a_o)\rho_o v_o - 2a_o b_o \lambda_o^\gamma \rho_o v_o. \]
\[ (2.95) \]
\[ (2.96) \]

The various coefficients and parameters in Equations (2.95) and (2.96) are given by

\[ a_w = \frac{\phi S_w \rho_w}{2\rho_w^e}, b_w = -\frac{\rho_w}{\rho_w^e}, c_w = \frac{(\rho_w^e + \phi S_w \Delta \gamma)\rho_w}{2\phi \rho_w^e}, \]
\[ a_o = \frac{\phi S_o \rho_o}{2\rho_o^e}, b_o = -\frac{\rho_o}{\rho_o^e}, c_o = \frac{(\rho_o^e + \phi S_o \Delta \gamma)\rho_o}{2\phi \rho_o^e}, \]

and

\[ \rho_w^e = \rho_w + \phi S_w \left[ \Delta \gamma - S_w \frac{\partial (\Delta \gamma)}{\partial S_w} \right], \]
\[ \rho_o^e = \rho_o + \phi S_o \left[ \Delta \gamma - S_w \frac{\partial (\Delta \gamma)}{\partial S_w} \right], \]
\[ \rho^e = \rho_w + \rho_o - \phi \left[ (S_o - S_w) \Delta \gamma + S_w S_o \frac{\partial (\Delta \gamma)}{\partial S_w} \right], \]
\[ \Delta \gamma = 2p_c(S_w) + \gamma_w - \gamma_o, \]
\[ \lambda^\gamma_l = \lambda \gamma_l. \]

The last issue remaining to be addressed is the relationship between physical system units and lattice system units. The conversion from lattice convection time
units (i.e., time needed for information propagation from cell to cell) to physical time units is straightforward. If \((N, L)\) and \((V, U)\) represent the characteristic lengths and absolute velocities for both the lattice and the physical system, we can relate the typical times \((t, T)\) for the evolution of both systems by

\[
\frac{t}{T} = \frac{N/L}{V/U}.
\]

Thus

\[
1 \text{ (physical time unit)} = \frac{N/L}{V/U} \text{ (lattice time unit)}.
\]

Consequently, \(\frac{N/L}{V/U}\) lattice time steps are equivalent to one physical time unit.

The pressure conversion depends on the real physical units used as well as the ratio of lengths and times if the form of Darcy's law in an absolute set of units is employed. With permeability, \(k\), in Darcy, viscosity, \(\mu\), in centipoise, and time, \(T\), in days, the conversion from psi to lattice pressure units is given by

\[
1 \text{ (psi)} = \frac{24 \times 3600}{30.48^2 \times 14.7} \frac{NV}{LU} \text{ (lattice pressure unit)}.
\]

### 2.4.3 Verification and testing

**Test case 1: The Buckley-Leverett problem.** The data for the Buckley-Leverett example are identical to those employed by Spivak et al (1977), so results may be compared. These data are given in Table 2.2.

The interstitial water saturation and residual oil saturation are assumed to be zero, and the relative permeabilities are quadratic in each of the phase saturations, that is:

\[
k_{rw} = S_w^2
\]

and

\[
k_{ro} = (1 - S_w)^2.
\]

The boundary conditions were as follows. Initially, \(S_w = 0\), \(Q\) cu ft/d water injected at \(x = 0\), and \(Q\) cu ft/d total fluid (oil and water) produced at \(x = L\). As is well known, the solution to the Buckley-Leverett equation under these conditions will consist of a shock followed by an expansion or rarefaction wave. Consequently, a self-sharpening behaviour is exhibited. Thus, if numerical diffusion creates small
Length of system, ft  1000
Porosity  0.10
Permeability, mD  157.977
Cross-sectional area, sq ft  1
Q (throughput) cu ft/sq ft/d  0.1
p_c, psi  0
Oil viscosity, cp  4
Water viscosity, cp  1

Table 2.2: Parameters for Buckley-Leverett Problem.

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![Diagram showing Buckley-Leverett problem](image)

Figure 2.18: Buckley-Leverett, one-dimensional waterflood example.
Figure 2.19: Saturation contours at 0.12 PVI early in the simulation for the benchmark run of a quarter five-spot waterflood.

Figure 2.20: Saturation contours at 0.57 PVI just before breakthrough, for the benchmark run of a quarter five-spot waterflood.
saturations ahead of the shock, a situation is created in which the waveform continually attempts to re-form. It is for this reason that the lattice Boltzmann solution with $p_c = 0$ converges to a solution different from the Buckley-Leverett solution. However, a simple way of ensuring convergence to a physical solution is to add extra dissipation by the introduction of a relatively small amount of capillary pressure, as shown by comparing the Lattice Boltzmann and finite-difference results for the case of $p_c = 3.0(1 - S_w)$ in Figure 2.18, where the Buckley-Leverett solution is shown along with the lattice Boltzmann solutions and the finite-difference solution. In the lattice Boltzmann solutions, the values $N = 200$ and $\nu = 0.0025$ have been used. The finite-difference solution with $N = 400$ shown in Figure 2.18 is marked “CMG-FD” and should be close to the true solution.

The finite-difference solution to this problem was obtained using the adaptive implicit-explicit (IMEX) black-oil simulator developed by the Computing Modeling Group (CMG) of Calgary. IMEX software is one of the most popular commercial reservoir simulators and can be used to model three-phase water/oil/gas systems or two-phase water/oil systems. The simulator includes the effects of gravity and ca-
Figure 2.22: Saturation contours at 720 days for an unfavourable mobility ratio and a diagonal-grid, five-spot waterflood.

Figure 2.23: Saturation contours at 1440 days for an unfavourable mobility ratio and a diagonal-grid, five-spot waterflood.
Figure 2.24: Saturation contours at 720 days for an unfavourable mobility ratio and a parallel-grid, five-spot waterflood.

Figure 2.25: Saturation contours at 1440 days for an unfavourable mobility ratio and a parallel-grid, five-spot waterflood.
Figure 2.26: Comparison of oil recovery curves computed for diagonal and parallel five-spot grids as pore volumes injected.

pillary pressure. It can run in one-, two- or three-dimensional modes. Variable grid spacing can be used. The nonlinear equations are solved by Newtonian iteration with the derivatives of the Jacobian matrix evaluated numerically. The simulator contains several possible options for the weighting of mobilities. These include single-point upstream, two-point upstream, and centralized upstream weightings. The time discretization is by backward differences with a modified Crank-Nicholson method included as an option. The well model permits the placing of wells at various positions in a grid block. Multiblock completion wells are included and are modeled in a manner which does not increase the matrix bandwidth. Finally, an efficient solution routine is included in the simulator. This routine provides Gaussian elimination and two different iterative solution methods. The simulator is fully implicit in its basic formulation. It becomes highly implicit, not fully implicit, when the options for two-point upstream or centralized upstream weightings are used or when multiblock completion wells are modeled.

For this problem the simulator was run in a two-phase, two-dimensional mode. The basic fully implicit formulation was used. The time discretization was backward
differences. The matrix problem was solved by the Gaussian elimination routine.

It is important to point out that the upstream (or upwind) techniques used in the IMEX simulator introduce a non-physical, artificial dissipation into the problem, whereas our lattice-Boltzmann solution introduces physical dissipation through the addition of a small capillary pressure term. Although the Buckley-Leverett problem is constantly referred to, it should be appreciated that it is idealized and, consequently, non-physical.

**Test case 2: Repeated five-spot pattern.** A series of runs were made for the five-spot problem with \( k = 157.997 \) md and \( \phi = 0.10 \). A 32 x 32 diagonal grid was used and no flow boundary conditions were specified along all boundaries. An injector with \( Q = 20 \) cu ft/d was located in the lower left corner and a producer with \( Q = 20 \) cu ft/d in the upper right corner.

The first run for this quarter five-spot problem is an academic unit-mobility ratio "benchmark" case, allowing comparison with an analytical solution. This benchmark run deals with "X-shape" relative permeability functions \( k_{rw} = S_w, k_{ro} = 1 - S_w \), respectively; no capillarity assumed. The corresponding analytical solution has been described by Morel-Seytoux (1965).

The positions of the saturation contours at 0.12 pore volume injected (PVI) are shown in Figure 2.19. It is seen that the saturation profile is smeared early in the simulation. In Figure 2.20 the positions of the saturation contours at 0.57 PVI, just before water breakthrough, are delineated. The computed breakthrough occurs at 0.60 PVI, which corresponds to a breakthrough areal sweep efficiency of 0.7. This figure compares favourably with the analytically derived value of 0.72 (Morel-Seytoux, 1965). The positions of the saturation contours at 0.67 PVI, just past the breakthrough, are indicated in Figure 2.21.

The second run of this five-spot problem was used to study the sensitivity of the lattice Boltzmann method to grid orientations. The distinction between a diagonal and a parallel grid is illustrated in Figure 2.7. For the parallel-grid case, a five-spot configuration has two injection wells and, therefore, two saturation fronts.

For this study, the relative permeabilities were defined as in Test case 1 but the capillary pressure was defined by \( p_c = 10(1 - S_w) \), while the water and oil viscosities were 1 and 4 cp, respectively. The computed saturation contours for diagonal (32 x
32) grids at 720 and 1440 days are shown, respectively, in Figures 2.22 and 2.23. Similarly, the saturation contours for parallel (45 x 45) grids at 720 and 1440 days are shown, respectively, in Figures 2.24 and 2.25. As these figures make clear, there is no significant grid-orientation sensitivity. The oil recovery as a function of pore volume injected is compared for both the parallel and diagonal grids in Figure 2.26.

2.4.4 Concluding remarks

A square lattice Boltzmann method has been defined, programmed and tested for the simulation of two-dimensional, incompressible, two-phase immiscible flow equations. The lattice Boltzmann method is typically considered as a second-order method. Consequently, significant reductions in the diffusion of sharp fronts and in sensitivity to grid orientation result as compared to low-order finite-difference schemes. It should be emphasized here that because there are no solid physical justification of Darcy's law for multiphase fluids, and moreover, because lattice Boltzmann methods are more physically meaningful than pure numerical methods, the approach proposed here is more complicated than the counterpart in miscible displacement processes. A possible alternative is to develop a lattice Boltzmann method based on porous media models obtained from the theory of mixtures (Bowen, 1982) which is more physically based, but not practical at present.
Chapter 3

Lattice–Boltzmann Simulations of Seismic Wave Propagation

3.1 Reviews of Seismic Simulation

There are two basic approaches to the analysis of seismic data. The first treats the earth as a black box and uses statistical communication theory to infer the spatial positions of the major discontinuities in the subsurface. The second postulates that the recorded seismogram can be idealized as a solution to a particular implementation of the wave equation, subject to appropriate initial and boundary conditions. The idea is to obtain a close fit between the excitation response of the subsurface model and the actual data. The modeling process involves the choice of a suitable numerical algorithm to simulate the wave equation under a given set of subsidiary conditions.

3.1.1 Principles of seismic exploration

Exploration seismology is based on the analysis of acoustic waves reflected from different rock layers in the earth's subsurface. Seismic energy (source), emitted into the subsurface, encounters discontinuities between the layers and is partially reflected back to the surface. The returning reflections are detected and their strengths and arrival times are recorded. After processing the recorded data for improved resolution and signal-to-noise ratio, geophysicists and geologists derive information from the result concerning the geologic substrata ("seismic interpretation"). The seismic
source may consist of dynamite (land), a hydraulic vibrator (land and marine) or compressed air (marine). The subsurface response is measured by a number of detector stations. Each detector station consists of a number of electrically connected single detectors ("field pattern"). The signal measured at one detector station is called a seismic trace. All traces related to one source position define one seismic shot record. Typically, there may be 256 traces in one shot record. The data from one seismic line consists of a number of seismic shot records (say several hundreds). In a two dimensional seismic survey the distance between adjacent seismic lines may be several kilometers. In a three dimensional seismic survey adjacent seismic lines may be as close as 50 m. There is a general tendency in the seismic industry to decrease shot and detector spacings, to decrease the length of field patterns and to increase the number of detector stations.

Until now, the nucleus of any seismic processing package consists of common mid-point (CMP) processing. This means that after "demultiplexing", correction for irregular surface conditions ("elevation and/or weathering problems") and attenuation of surface waves ("groundroll problem") et al., the data is re-ordered such that all traces with the same mid-point between source and detector position are grouped in one gather, the so-called common mid-point gather (CMP gather). The arrival times of the reflections from one reflector in one CMP gather can be well approximated by a hyperbolic relationship,

\[ t_{k,n}^2 = t_k^2 + \frac{(2n\Delta h)^2}{v_{st}(t_k)} \]

where \( t_k \) is the zero-offset \((n=0)\) reflection time of the \( k^{th} \) reflector and \( h_n = 2n\Delta h \) represents the distance ("offset") between source and detector of the \( n^{th} \) trace in the CMP gather under consideration; \( v_{st}(t_k) \) is the so-called stacking velocity for the \( k^{th} \) reflector. Using a multi-trace coherency criterion, \( v_{st} \) is determined for a number of reflecting boundaries. From these values, interval velocities, for the layers in between these boundaries, can be computed. In general, prior to the velocity analysis, the CMP gather is treated by prediction-error filtering to achieve some pulse compression and to attenuate multiple reflections, reverberations and narrow band noise. The arrival times of all traces within this CMP gather are then corrected through \( t_{k,n} \rightarrow t_k \), such that the normal travel time effect of the offset ("move out") is eliminated ("NMO correction"). Finally, all NMO-corrected traces are added together to form one stacked trace. In
this way a considerable improvement in signal-to-noise ratio may occur and, last, but not least, a significant data reduction has been achieved. A stacked trace is considered to be a zero-offset trace and all stacked traces of a seismic line define a stacked or zero-offset section. After post-stack processing such as deconvolution and migration, stacked sections form the basic input data for seismic interpretation.

Without question, most of the recent advances in seismic exploration techniques have been made possible by new digital technology. This holds true in all three seismology areas – acquisition, processing and interpretation. The ability to record and store ever-growing volumes of seismic data, the ability to reduce noise on the recordings and then improve vertical and lateral resolution properties throughout large data sets, and finally the ability to manipulate vast quantities of data with advanced algorithms to arrive at ever more sophisticated and complex subsurface interpretations have all been made possible by improved digital technology. And as seismic exploration techniques continue to expand, items such as optical disks, and parallel computers will be taken for granted as everyday equipment in the exploration world. Integrated seismic-geologic interpretation, rapidly becoming an everyday occurrence, also owes its success to the digital technology revolution, especially workstation technology. Particularly during interpretation, whereby seismic information is extracted and presented such that it can be translated into detailed geologic information, the capabilities of workstations are essential. This is true in structure, stratigraphic and lithologic interpretation.

3.1.2 Derivation of the elastic wave equation

In the last few years the role of wave theory in seismic processing has increased significantly; new wave theory solutions have been formulated to old problems with impressive success. In the near future the technology of seismic processing will largely be based on wave theory. This means that in the coming years emphasis will further shift from time-sequence-based techniques to wave-theory-based techniques. A rigorous derivation of the full elastic wave equation for an inhomogeneous, anisotropic solid is presented by many authors (i.e., Achenbach, 1973; Pilant, 1979; Aki and Richards, 1980). Here we only present a summary and emphasis on the similarity between the Navier-Stokes equation of a viscous flow and the elastic wave of a solid from con-
tinuum mechanics point of view, partly because such a treatment is lacking in books on seismology.

In continuum mechanics, there are two common laws for mass and momentum. They are equations of continuity and motion. The equation of continuity may be written as

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0,
\]

where \(\rho\) is the local density of the medium, \(\mathbf{v}\) is the local mass average velocity. The equation of linear momentum for a continuous medium may be written as

\[
\frac{\partial (\rho \mathbf{v})}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) = \nabla \cdot \mathbf{\Pi} + \rho \mathbf{f},
\]

where the pressure or stress \(\mathbf{\Pi}\) is a second-rank tensor (dyadic) and \(\mathbf{f}\) is the external body force per unit mass. These two equations are applicable to any continuous medium. However, they are insufficient to fully characterize the behavior of the medium because they do not distinguish between different types of materials. For a Newtonian fluid, we have the following relation,

\[
\mathbf{\Pi} = -p\mathbf{I} + \left(\kappa - \frac{2}{3}\mu\right) (\nabla \cdot \mathbf{v}) \mathbf{I} + \mu (\nabla \mathbf{v} + \mathbf{v} \nabla),
\]

where \(p\) is the hydrostatic pressure; \(\mathbf{I}\) is the unit tensor, \(\kappa\) is the bulk or volume viscosity, sometimes written as \(\lambda + \frac{2}{3}\mu\); \(\mu\) is the shear viscosity; and \(\mathbf{v} \nabla\) is the transpose of \(\nabla \mathbf{v}\). Substitution of the resulting expression for \(\mathbf{\Pi}\) into Equation (3.2) ultimately gives the following general equation of motion for a Newtonian fluid,

\[
\frac{\partial (\rho \mathbf{v})}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) = -\nabla p + \nabla [(\kappa - \frac{2}{3}\mu)(\nabla \cdot \mathbf{v})] + \nabla [\mu (\nabla \mathbf{v} + \mathbf{v} \nabla)] + \rho \mathbf{f},
\]

This equation, along with the equation of state \(p = p(\rho, T)\), the density dependence of shear viscosity \(\mu = \mu(\rho, T)\), the density dependence of bulk viscosity \(\kappa = \kappa(\rho, T)\), and the boundary and initial conditions, determines completely the pressure, and velocity components of a flowing isothermal fluid. Equation (3.4) is not usually used in its complete form, but rather is specialized for individual flow problems. Thus, \(\kappa\) is often taken equal to zero. Substitution into Equation (3.4), reduces to the Navier-Stokes equation.

\[
\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) = -\nabla p + \nabla (\mu \nabla \mathbf{v}) + \rho \mathbf{f}.
\]
Now let us specialize the equation of motion to small displacements of a linear elastic solid. The most common form of Hooke's law is written as,

$$\mathbf{\Pi} = (\lambda + \frac{2}{3} \mu)(\nabla \cdot \mathbf{u})\mathbf{I} + \mu[\nabla \mathbf{u} + \mathbf{u} \nabla - \frac{2}{3}(\nabla \cdot \mathbf{u})\mathbf{I}].$$

(3.6)

where \( \mathbf{u} \) is the displacement. \( \lambda \) and \( \mu \) are known as the Lamé coefficients or Lamé moduli. We call \( \mu \) the rigidity or shear modulus and \( \kappa = \lambda + \frac{2}{3} \mu \) the bulk modulus. Now we need merely insert the elastic stress tensor to obtain the general equation of motion. Under the assumptions of small displacement, we make the approximations.

$$\mathbf{v} = \frac{\partial \mathbf{u}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{u} \simeq \frac{\partial \mathbf{u}}{\partial t},$$

(3.7)

$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} \simeq \frac{\partial^2 \mathbf{u}}{\partial t^2}.$$  

(3.8)

Under these conditions, Equation (3.2) reduces to Cauchy's equation of motion for the infinitesimal theory of elasticity.

$$\rho \frac{\partial^2 \mathbf{u}}{\partial t^2} = \nabla \cdot \mathbf{\Pi} + \rho \mathbf{f}.$$  

(3.9)

The equation of continuity, Equation (3.1), leads us to,

$$\frac{\delta \rho}{\rho} = -\nabla \cdot \mathbf{u}.$$  

(3.10)

In problems pertaining to elastic wave propagation in the solid earth, the density changes because of the wave motions are small. When the Hooke's law is added, the dynamic equation of an elastic medium in the presence of external forces \( \rho \mathbf{f} \) thus follows as,

$$\rho \frac{\partial^2 \mathbf{u}}{\partial t^2} = \nabla[\kappa(\nabla \cdot \mathbf{u})] + \nabla(\mu \nabla \mathbf{u}) + \rho \mathbf{f}.$$  

(3.11)

or

$$\rho \frac{\partial^2 \mathbf{u}}{\partial t^2} = \nabla \left(\frac{1}{3} tr \mathbf{\Pi}\right) + \nabla(\mu \nabla \mathbf{u}) + \rho \mathbf{f}.$$  

(3.12)

with

$$\frac{1}{3} tr \mathbf{\Pi} = -\frac{\kappa}{\rho} \delta \rho.$$  

(3.13)

This should be compared with Equation (3.5) for a viscous fluid. Here, it appears that the average tensile stress in solids \( \frac{1}{3} tr \mathbf{\Pi} \) plays the same role as the negative pressure in fluids. Moreover, although both equations involve the acceleration \( \rho \frac{dv}{dv} \), the viscous
stress (3.5) depends on the time rate of change of the strain, introducing second spatial
derivatives of \( \mathbf{v} \), in contrast to the more familiar second spatial derivatives of \( \mathbf{u} \) seen
in Equation (3.12).

Considering the simplest case of wave propagation in a homogeneous medium, we
take \( \rho, \lambda \) and \( \mu \) to be constant in the elastic wave equation and ignore the external
force to give

\[
\rho \frac{\partial^2 \mathbf{u}}{\partial t^2} = (\lambda + \mu) \nabla (\nabla \cdot \mathbf{u}) + \mu \nabla^2 \mathbf{u}.
\]  

(3.14)

To interpret this relation, we shall separate the general vector field \( \mathbf{u} \) into its longitudi-
dinal and transverse components,

\[
\mathbf{u} = \mathbf{u}_l + \mathbf{u}_t
\]

(3.15)

where

\[
\nabla \times \mathbf{u}_l = 0, \quad \nabla \cdot \mathbf{u}_t = 0.
\]  

(3.16)

Note that \( \mathbf{u}_t \) is a pure shear distortion with no change in volume, whereas \( \mathbf{u}_l \) in-
volves compression and rarefaction. Substitution of Equations (3.15) and (3.16) into
Equation (3.14) and use of the vector identity

\[
\nabla^2 \mathbf{u} = -\nabla \times (\nabla \times \mathbf{u}) + \nabla (\nabla \cdot \mathbf{u})
\]

(3.17)
effects a separation of Equation (3.14) into two wave equations, one governing the
dilatation (volume changes)

\[
\frac{1}{v_p^2} \frac{\partial^2 \mathbf{u}_l}{\partial t^2} = \nabla^2 \mathbf{u}_l,
\]

(3.18)

with speed

\[
v_p = \sqrt{\frac{\lambda + 2\mu}{\rho}}
\]

(3.19)
and the other rotation

\[
\frac{1}{v_t^2} \frac{\partial^2 \mathbf{u}_t}{\partial t^2} = \nabla^2 \mathbf{u}_t,
\]

(3.20)
with speed

\[
v_s = \sqrt{\frac{\mu}{\rho}}.
\]

(3.21)
Change in volume is an essential feature of P waves while rotation is an essential
feature of S waves. For normal materials \( v_p > v_s \), implying that P waves are the faster
of the two and will therefore arrive first.
3.1.3 Numerical modeling techniques

Numerical modeling techniques for seismic wave propagation can be grouped into three categories – analytical, semianalytical and numerical methods. Analytic methods, including Cagniard-de Hoop, Wiener-Hopf (Bouwkamp, 1954; de Hoop and van der Hijden, 1983) and other integral transform techniques, involve no approximation other than the original idealization of the problem. While these methods give a great deal of physical insight about how seismic events arise, analytical methods are at present limited to the most simple geometries amenable to separation of variable techniques. Though restricted to simple geologies, analytic methods can give the solution for the entire parameter space of velocity, density and layer thickness. The application of analytic modeling techniques to wave equation based processing is limited to those same separable geometries as the forward modeling problem, such as 1-D wave equation inversion using the method of characteristics (Gray, 1980).

Semianalytic solutions, including asymptotic ray and Gaussian beam theories give only approximate (usually high frequency) solutions to the wave equation. The typical implementation involves solving a simplified wave equation in smoothly varying media, such as the eikonal and transport equations in asymptotic ray theory or perhaps a parabolic one-way equation in Gaussian beam theory. At discrete interfaces one explicitly applies reflection, transmission, diffraction, head wave and surface wave coefficients obtained by the asymptotic analytic solution of a simpler subproblem involving only two media and the interface in question. In principle, semianalytic methods can be generalized to give arbitrarily accurate results by increasing the number of terms retained in the Kline-Luneberg frequency expansion (Gjoystdal and Ursin, 1984) and by increasing the number of multiple reflection and refraction events used in creating the synthetic. Such a generalization can become prohibitively expensive and could produce divergent solutions. Furthermore, diffraction, head wave and surface wave coefficients have been worked out for only the lowest order terms of the Kline-Luneberg expansion. Because analytic solutions are used at discontinuities, each event can be tagged by its polarization and whether it is a direct wave, a reflection, a refraction, a head wave, a diffraction, a surface wave, a multiple or a converted wave.

Numerical methods include finite differences, finite elements, boundary integral equations and spectral methods. In general, all these methods can model arbitrarily
complicated two and three-dimensional media with irregular interfaces, though it is an understatement to say that three-dimensional elastic modeling can be quite expensive for all but the simplest (simple now meaning small) models at the present time. One can model arbitrary source and receiver polarization, as well as corresponding array design. In contrast to semianalytic methods, the numerical methods give accurate solutions for the entire wave field, but little or no insight into event identification. In addition, while numerical algorithms may cost more to run than semianalytic algorithms for simple geologies, the numerical algorithms are easier to code and maintain than the semianalytic algorithms. Seismologist began using finite difference methods to solve wave propagation problems some 25 years ago (Alterman and Kornfeld, 1968). Production finite difference codes in seismic modeling today are almost exclusively explicit time marching schemes (Mufti, 1985). The more flexible forms use either an inhomogeneous formulation of the second order system of equations on a single grid (Boore, 1972; Kelly et al., 1976) or by solving the first order system of equations on two staggered grids (Madariaga, 1976; Virieux, 1984; Virieux, 1986; Levander, 1988). The use of high-order operators (Dablain 1986; Shubin and Bell, 1987) permits the use of coarser grids and results in a potentially more efficient algorithm, since CPU time and I/O time may be more closely balanced. This idea leads to the coarse grid pseudospectral (Fourier transform) methods (Orszag, 1972; Gazdag, 1981: Kosloff and Baysal, 1982). In comparison to finite differences, there is little published work on the finite-element solution specific to seismic exploration problems. Most of them are used to tackle more difficulty problems, including topographic related problems. Hybrid schemes which combine finite-difference or finite element methods with boundary element methods can be very attractive when the heterogeneous part of the model is confined to a limited region (Kummer et al., 1987; Van den Berg, 1987). A through review of numerical modeling for seismic wave propagation is given by Kelly and Marfurt (1990).

3.2 Acoustic Wave Modeling

The lattice-gas based cellular automaton fluid method has been presented as a fast and efficient way for solving seismic acoustic wave equations (Rothman, 1987; Huang et al,
1988). However, there exist some fundamental problems in this method in modeling wave propagation in a realistic earth model. Besides its intrinsic noisy character which make the computational accuracy difficult to achieve, one of the most serious disadvantages is the difficulty of extending the models from homogeneous to general inhomogeneous media. As a result, its possible advantage over other conventional computational methods is greatly obscured. Unless these problems are resolved, the lattice-gas based cellular automaton fluid methods can hardly be used as a useful tool for numerical seismic modeling or imaging.

The current trend in cellular automaton fluid simulation is to replace the lattice-gas approach with the lattice Boltzmann approach (McNamara and Zanetti, 1988; Higuera et al, 1989). The lattice Boltzmann approach shares with cellular automaton models the efficiency of local operations, discrete structure, and ease of parallelization, but uses a real-number description for the particle distribution and ignores particle-particle correlation completely, consequently, requiring, relative to cellular automaton, many fewer lattice-sites and maintaining a higher signal-to-noise ratio. By allowing for an infinite number of possible states and collisions per site, the lattice Boltzmann approach allows independent specification of the parameters of the equilibrium distribution as well as a great deal of latitude in the choice of its function form. There is enough freedom to construct both an equilibrium distribution and a collision operator to describe acoustic wave propagation in general inhomogeneous media. In addition, whereas much of the computational effort in cellular automaton fluid dynamics is involved in the evaluation of complex Boolean collision operators, the lattice Boltzmann approach affords additional efficiency due to flexibility in handling collision terms, particularly by using a BGK relaxation scheme (Qian et al, 1992). There exists a different lattice Boltzmann acoustic wave model (Mora, 1992; Huang and Mora, 1993) which differs from the traditional lattice Boltzmann scheme in replacing the stream process by either finite difference or interpolation schemes. Consequently, this model reduces the level of computational efficiency of lattice Boltzmann methods. In addition, there are difficulties to handle sharp interfaces.

In this section we first describe the lattice Boltzmann acoustic model, and then present simple one-dimensional and two-dimensional examples which demonstrate its convergence and precision.
3.2.1 Lattice Boltzmann acoustic model

Seismic P-waves can be approximated by the following linear acoustic wave equation of continuity and momentum under the assumption of small-amplitude perturbations to the static state (Wapenaar and Berkhout, 1989),

\[
\frac{\partial [\Delta \rho(x, t)]}{\partial t} + \rho_0(x) \nabla \cdot \mathbf{v}(x, t) = 0, \tag{3.22}
\]

\[
\rho_0(x) \frac{\partial \mathbf{v}(x, t)}{\partial t} + \nabla [\Delta p(x, t)] = 0, \tag{3.23}
\]

\[
\Delta p(x, t) = c_s^2 \Delta \rho(x, t), \tag{3.24}
\]

where \( \rho_0(x) \) and \( \rho_0(x) \) represent the static pressure and mass density, respectively; \( \Delta p(x, t) \) and \( \Delta \rho(x, t) \) represent the pressure and mass density changes caused by the acoustic wave field, respectively, and \( c_s \) is referred to as the speed of sound. Note that Equations (3.22)-(3.24) can be obtained by setting \( \mu = 0 \) (ideal fluids) in Equations (3.10), (3.11) and (3.13). In the following we will introduce a lattice Boltzmann equation scheme that can simulate the linear acoustic equation above.

In the lattice Boltzmann method, the kinetic evolution equation for the equal-mass-particle distribution \( f_i(x, t) \) can be written as follows.

\[
f_i(x + \mathbf{e}_i \Delta t, t + \Delta t) = f_i(x, t) + \Omega_i(f(x, t)). \tag{3.25}
\]

where \( \Omega_i(f(x, t)) \) is a local collision operator depending on local particle distribution \( f_i(x, t) \) only. The velocity vectors \( \{ \mathbf{e}_i; i = 0, 1, \cdots, b \} \) are the possible velocities a particle can have in order to move from a lattice site to one of the \( b \) numbers of the nearest neighboring site at each time step. \( |\mathbf{e}_0| = 0 \) is associated with the rest ("stopped") particles, and \( |\mathbf{e}_i| = c (i = 1, \cdots, b) \), where \( c = \frac{\Delta x}{\Delta t} \), is associated with the moving particles. For simplicity, we adopted a "single relaxation time" form for the collision operator (Qian et al. 1992)

\[
\Omega_i(x, t) = -\frac{1}{\tau} [f_i(x, t) - f_i^{eq}(x, t)]. \tag{3.26}
\]

where \( \tau \) is the mean collision time and determines its fluid viscosity. \( f_i^{eq}(x, t) \) is the equilibrium distribution with a given functional form at site \( x \) and time \( t \). A H theorem can be proved for this system for arbitrarily given form of \( f_i^{eq}(x, t) \), as long as this equilibrium distribution function is positive (Qian et al. 1992).
In order to derive the macroscopic hydrodynamic equations, the Chapman-Enskog procedure is utilized, assuming the following multi-scale expansion of the time and space derivatives in the small parameter, \( \epsilon \):

\[
\frac{\partial}{\partial t} = \epsilon \frac{\partial}{\partial t_1} + \epsilon^2 \frac{\partial}{\partial t_2} + \cdots, \\
\nabla = \epsilon \nabla_1 + \epsilon^2 \nabla_2 + \cdots.
\]

(3.27)  

(3.28)

We also expand the distribution as

\[
f_i = f_i^{(0)} + \epsilon f_i^{(1)} + \epsilon^2 f_i^{(2)} + \cdots,
\]

(3.29)

where the zeroth-order term is the equilibrium distribution, so that the collision operator becomes

\[
-\frac{(f_i - f_i^{eq})}{\epsilon \tau} = -\frac{1}{\tau} (f_i^{(1)} + \epsilon f_i^{(2)} + \cdots).
\]

(3.30)

Note that the parameter \( \epsilon \) can be regarded as a Knudsen number similar to kinetic theory in classical statistical mechanics. Since the fluid mass, \( \rho \), and the momentum, \( \rho \mathbf{v} \), are conserved in collisions:

\[
\rho = m \sum_i f_i = m \sum_i f_i^{(0)},
\]

(3.31)

\[
\rho \mathbf{v} = m \sum_i f_i \mathbf{e}_i = m \sum_i f_i^{(0)} \mathbf{e}_i,
\]

(3.32)

where \( m \) is the particle unit mass. the summations over nonequilibrium populations are zero: \( \sum_i f_i^{(l)} = 0 \) and \( \sum_i \mathbf{e}_i f_i^{(l)} = 0 \) for \( l > 0 \).

Substituting the above expansions (3.27)-(3.30) into the kinetic equation (3.25), we obtain equations of first and second order in \( \epsilon \) which are written as

\[
\frac{\partial}{\partial t_1} f_i^{(0)} + \mathbf{e}_i \cdot \nabla_1 f_i^{(0)} = -\frac{1}{\tau} f_i^{(1)},
\]

(3.33)

and

\[
\frac{\partial}{\partial t_2} f_i^{(0)} + \left( \frac{\partial}{\partial t_1} + \mathbf{e}_i \cdot \nabla_1 \right) (1 - \frac{1}{2\tau}) f_i^{(1)} = -\frac{f_i^{(2)}}{\tau}.
\]

(3.34)

where \( \tau \) is assumed to be \( O(1) \).

When Equations (3.33) and (3.34) are summed over the \( i \) velocities, the continuity or mass conservation equation to second order in \( \epsilon \) is

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0.
\]

(3.35)
The momentum equation to second order in $\epsilon$ is obtained by multiplying the above equations by $e_i$ and then summing over velocities,

$$\frac{\partial}{\partial t}(\rho v) + \nabla \cdot \Pi = 0,$$  \hspace{1cm} (3.36)

where $\Pi$ is the momentum flux tensor, defined as

$$\Pi_{\alpha\beta} = m \sum_i e_{i\alpha} e_{i\beta} \left[ f_i^{(0)} + (1 - \frac{1}{2\tau}) f_i^{(1)} \right],$$  \hspace{1cm} (3.37)

Note that the factor $\frac{1}{2\tau}$ comes from the second time and space derivatives.

The constitutive relations for this tensor are obtained by selecting a particular lattice geometry and equilibrium distribution functional form and then proceeding to match moments of the distribution with terms in the nonlinear or linear acoustic equation of motion.

For the purpose of recovering linear acoustic equations (3.22)–(3.24), here we use a 5-velocity square lattice with moving velocities, $e_i = c(\cos \frac{(i-1)\pi}{2}, \sin \frac{(i-1)\pi}{2})$ for $i = 1, \cdots, 4$ in a two dimensional model. The extension of this model to a three dimensional one is straightforward. A suitable equilibrium distribution is found to be

$$f_0^{eq} = \alpha \frac{\rho}{m},$$  \hspace{1cm} (3.38)

$$f_i^{eq} = \frac{1}{4} \frac{\rho}{m} (1 - \alpha + 2 \frac{e_i \cdot \mathbf{v}}{c^2}).$$  \hspace{1cm} (3.39)

Substituting Equations (3.38) and (3.39) into (3.37) for $\Pi$ above and ignoring the second order term by setting the mean collision time $\tau$ close to $\frac{1}{2}$, we find that

$$\Pi_{\alpha\beta} = \frac{1 - \alpha}{2} c^2 \rho \delta_{\alpha\beta}.$$  \hspace{1cm} (3.40)

The (isothermal) sound speed, therefore, is given by identifying the isotropic part of this tensor with the pressure, through

$$c_s^2 = \frac{1 - \alpha}{2} c^2.$$  

Upon substitution Equation (3.40) into (3.36), the final form of the momentum equation is

$$\frac{\partial}{\partial t}(\rho v) + \nabla(c_s^2 \rho) = 0.$$  \hspace{1cm} (3.41)
To obtain the linear acoustic equation, considering a weak perturbation of the equilibrium solution with density \( \rho_0 \) and pressure \( p_0 \), we define,

\[
p(x, t) = p_0(x) + \Delta p(x, t),
\]

and

\[
\rho(x, t) = \rho_0(x) + \Delta \rho(x, t),
\]

where \( \Delta \rho \) and \( \Delta p \) represent the pressure and density changes caused by the acoustic wave field.

With these assumptions, we obtain from Equations (3.35) and (3.41) the linear equations of continuity and momentum, respectively,

\[
\frac{\partial (\Delta \rho)}{\partial t} + \nabla \cdot (\rho_0 \mathbf{v}) = 0,
\]

\[
\rho_0 \frac{\partial \mathbf{v}}{\partial t} + \nabla (\Delta p) = -\nabla K,
\]

\[
\Delta p = c_2^2 \Delta \rho.
\]

where \( K = c_2^2 \rho_0 \) is the adiabatic compression modulus.

Comparing the equations above and the linear acoustic equations (3.22)–(3.24), there is a term, \( -\nabla K \), in the second equation above that is not in the linear acoustic equations unless we have a homogeneous media where \( \nabla K = 0 \). In order to get rid of this unwanted term in inhomogeneous media, we add another nonlocal interaction collision operator to Equation (3.25)

\[
\Omega^{add}_i(x, t) = \frac{1}{2} \frac{K(x + e_i) - K(x)}{mc^2}.
\]

It is easy to verify that \( \sum_i \Omega^{add}_i(x, t) \sim 0 \) and \( \sum_i e_i \Omega^{add}_i(x, t) \sim \nabla K(x) \) when \( c \sim 0 \). Note that in a homogeneous region (a site where the compression modules of all the nearest neighbour sites are identical) of our linear acoustic wave model, the added collision operator, \( \Omega^{add}_i(x, t) \), is 0, and thus only has contribution in an inhomogeneous region. The physical interpretation of this term is as follows: When applied to material discontinuity, the equation of motion yields an additional body-force term. It is this term that guarantees the traction continuity. The heterogeneous lattice Boltzmann scheme resembles in this respect, the seismic-source modeling by means of body-force equivalents. Instead of prescribing the displacement discontinuity at a fault plane, a body-force term is added to the equation of motion.
The scheme described above cannot be used at the boundary of the lattice unless special provisions are made. The problem is that a node at the boundary cannot gather the incoming particles from a non-existent neighbour. However, in the real wave propagations the behaviour at the boundary is defined by its boundary conditions. Examples of some boundary conditions in seismic modeling are the free surface and absorbing boundary conditions. The basic idea for this technique is to derive a relation between the incoming particles and outgoing particles from the given boundary conditions. Consider a velocity direction \( i \) from a missing neighbour site into the wave field area. Let \( f_i^{\text{IN}} \) denote the incoming particle distribution along \( e_i \) and \( f_i^{\text{OUT}} \) the outgoing particle distribution along \(-e_i\). Now using Equation (3.39) the following relations between \( f_i^{\text{IN}} \) and \( f_i^{\text{OUT}} \) can be derived

\[
\begin{align*}
  f_i^{\text{IN}} + f_i^{\text{OUT}} &= \frac{1 - \alpha \rho}{2} \frac{m}{v}, \\
  f_i^{\text{IN}} - f_i^{\text{OUT}} &= \frac{\rho}{m} e_i \cdot \frac{v}{c^2}.
\end{align*}
\]

The first equation shows immediately how, in general, pressure (or density) boundary conditions can be imposed. A special case of a pressure boundary condition is the free surface where \( \Delta p = 0 \) (or \( \rho = \rho_0 \)) and

\[
f_i^{\text{IN}} = \frac{1 - \alpha \rho_0}{2} \frac{m}{v} - f_i^{\text{OUT}}
\]

To implement an absorbing boundary condition, for example, the condition B-1 of Clayton and Engquist (1977),

\[
\frac{\partial (\Delta p)}{\partial t} = c_s \frac{\partial (\Delta p)}{\partial x}.
\]

Upon substitution into Equation (3.22), we obtain an approximation to the particle velocity estimate

\[
\rho_0 v(x, t) = \rho_0 v(x + e_i \Delta t, t) + \frac{c_s}{\rho_0} [\rho(x, t) - \rho(x + e_i \Delta t, t)],
\]

where \( \rho \) and \( v \) are calculated according Equations (3.31) and (3.32). Applying this to (3.49), \( f_i^{\text{IN}} \) may be obtained.

### 3.2.2 Numerical Examples

To investigate the convergence of the proposed lattice Boltzmann equation method for acoustic waves, a representative test case was formulated in one-dimension. The
Figure 3.1: One-dimensional model for numerical convergent tests.

The velocity model used for this study is illustrated in Figure 3.1. The distance from the source to the farthest receiver is 5203 m. The total model is 10406 m long. All other parameters of significance are listed in Figure 3.1.

Figure 3.2 shows the time windows for the primary arrivals at receivers 1, 2, and 3 which were generated at three different grid samplings, 10.16 m, 5.08 m, and 2.54 m. That the lattice Boltzmann equation solution does indeed converge on the analytical result is verified by realizing that the solution of the 1-D wave equation with a source is the first integral of the source shifted by \( x = c_s t \) (Chester, 1971). Figure 3.3 shows the first integral of the Ricker wavelet source, which was computed from its analytical expression. It agrees very well with the wave recorded at receiver 1 with the finest grid sampling. Receivers 2 and 3 should, in theory, be the input wave multiplied by the transmission coefficient, which in this case is 4/3. Again, the results on the finest grid at receivers 2 and 3 show good agreement with the expected theoretical result. These considerations justify the convergence of the lattice Boltzmann equation method, and, consequently, use of this experiment as a comparative study to investigate the
Figure 3.2: Numerical solutions of 1-D model for the primary arrivals at receivers 1, 2, and 3 which were generated at three different grid samplings, 10.16 m, 5.08 m and 2.54 m.
Figure 3.3: The first integral of the Ricker wavelet, confirming the free-space solution of the 1-D wave equation as an integration of the source.

The relative performance of the lattice Boltzmann equation method with the second-order and fourth-order finite difference algorithms. Dablain (1986) has computed arrivals from the same model at receivers 1, 2 and 3 on the grid of $\Delta x = 10.16m$. Comparison of Figure 3.2 and Figures 4 and 6 in Dablain’s paper shows that the results from the lattice Boltzmann method are close to the one from the fourth-order finite difference method. This suggests that the relative performance of the lattice Boltzmann approach is more or less equivalent to a fourth-order differencing scheme rather than second-order schemes.

The accuracy of the lattice Boltzmann equation method was also tested for a more realistic 2-D wave propagation in a structure that contains a single uniform layer overlying a homogeneous half-space. Although this problem appears simple, it poses a serious challenge to forward modeling methods because it contains post-critical-angle phenomena, high velocity contrasts and reflections from the free surface. In addition, because this problem possesses an analytical solution, it has long been served as a
Figure 3.4: Configuration of 2-D acoustic layer model.

test of the accuracy of numerical methods. In the present example, the configuration of the problem is shown in Figure 3.4. The velocities of the layer and half-space were 2 km/s and 4 km/s, respectively. The uniform density was chosen equal to unity. The layer thickness was 1 km. The source was located at a depth of 800 m beneath the free surface and had a Ricker wavelet time history. The dominant frequency of the wavelet was 25 Hz which corresponds to a wavelength of $10\sqrt{2}$ grid points in the low velocity region. The calculations used a grid size of 443 x 443 with horizontal and vertical grid spacings of $4\sqrt{2}$ m. The numerical solution was propagated to 1.6 s in increments of 1 ms.

Figures 3.5(a–c) show amplitude snapshots at $t=0.4$ s, $t=0.8$ s and $t=1.2$ s, respectively. The numbered events in the figures are interpreted as the direct arrival (1), the reflected arrival (2), the surface multiple (3) and two reflected multiples (4) and (5). There are noticeable arrivals from the corners at the top boundary in the snapshot at $t=1.2$ s. Otherwise, the absorbing boundary works very well. This is because the effectiveness of condition (3.51) is restricted to waves impinging at the boundary.
Figure 3.5: Amplitude snapshots at 0.4s, 0.8s and 1.2s, respectively. Numbered events correspond to direct wave (1), reflected wave (2), surface multiple (3), reflected multiples (4) and (5), transmitted wave (8), head wave (9) and transmitted multiple (10).

at oblique or small angles. A high-order radiation boundary can be implemented by deriving a more involved relation between $f_i^{IN}$ and $f_i^{OUT}$ if necessary.

A more accurate evaluation of the numerical results is given by comparing known analytical solutions. Figures 3.6(a–c) show time histories at three locations at a depth of 250 m and at horizontal distance from the source of 0 m, 600 m and 750 m, respectively; corresponding to precritical, about critical and post-critical distances with respect to the layer reflection. The analytical solutions for events (1)–(5), based on the modified Cagniard technique (Drijkoningen and Fokkema, 1987), are shown in solid line in Figure 3.6, whereas the numerical solutions are shown in dashed lines. The agreement between numerical and analytical solutions is very good except the reflections from the corners at the top boundary.
Figure 3.6: Comparison between analytical (solid) and numerical (dashed) solution for stations at a depth of 250 m and at horizontal distance from the source of 0 m, 600 m and 750 m respectively.
3.2.3 Concluding remarks

We have developed a lattice Boltzmann scheme for simulation of acoustic wave propagation in inhomogeneous media. The kinetics of this model can be easily implemented on a parallel architecture computer. We have demonstrated theoretically and numerically that the macroscopic behavior of this model corresponds to that of a linear acoustic equation. Experiments performed on serial computers have indicated that the lattice Boltzmann scheme has a better relative performance than the second-order central-differencing scheme though it is typically considered to be a second-order method. Successful implementation of boundary conditions, in particularly the free-surface boundary conditions, without padding extra rows or columns has suggested that the lattice Boltzmann method is probably a good method for modeling wave propagation in very complicated media, such as including inclusions and cracks (see Section 4.3).

3.3 Elastic Wave Modeling

The common assumptions made to simplify the elastic wave equation are frequently invalid for studying wave propagation in the earth. These assumptions include high-frequency approximations, flat-lying media, and coincident sources and receivers. Numerical methods such as finite difference, finite element, or spectral method are becoming increasingly popular in obtaining solutions to the elastic wave equation without making these assumptions. However, a frequently encountered problem is one where the media are strongly heterogeneous and these classical methods, which approximate the continuous derivatives of the differential equation by discrete operators, may become inaccurate or unstable. In hydrodynamics, lattice gas and lattice Boltzmann methods overcome similar numerical difficulties by simulating a microscopic equation of particle motion such that the energy and momentum are conserved. When viewed macroscopically, the lattice gas and lattice Boltzmann methods yield the same result as the desired differential equation (because the same quantities are conserved). Unfortunately, there is no presently known lattice gas or lattice Boltzmann models for elastic waves, the majority of lattice gas and lattice Boltzmann researchers having focused on the fluid flow whose dynamics are described by the Navier-Stokes equations. However, in Section 3.1 we have shown the similarity between the Navier-Stokes
equation of hydrodynamics and the wave equation of elastic solids. We believe there is no fundamental difference between these two equations. In other words, we could develop a lattice gas or lattice Boltzmann model for elastic waves, which are supported by the success of our lattice Boltzmann model for acoustic waves. This section will be dedicated to this attempt.

3.3.1 Numerical method

Consider the wave equation for P-SV waves. For waves with polarization in the vertical xz-plane the relevant components of the stress displacement relation (3.6) read,

\[
\sigma_{xx} = (\lambda + 2\mu) \frac{\partial u_x}{\partial x} + \lambda \frac{\partial u_z}{\partial z},
\]

(3.53)

\[
\sigma_{xz} = \mu \left( \frac{\partial u_x}{\partial z} + \frac{\partial u_z}{\partial x} \right),
\]

(3.54)

\[
\sigma_{zz} = \lambda \frac{\partial u_x}{\partial x} + (\lambda + 2\mu) \frac{\partial u_z}{\partial z},
\]

(3.55)
whilst the relevant components of the equation of motion (3.9) read,

\[
\rho \frac{\partial^2 u_x}{\partial t^2} = \frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xz}}{\partial z} + \rho f_x, \quad (3.56)
\]

\[
\rho \frac{\partial^2 u_z}{\partial t^2} = \frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{zz}}{\partial z} + \rho f_z. \quad (3.57)
\]

In vector form, similar to Equations, (3.11)–(3.13)

\[
\frac{\partial \delta \rho(x,t)}{\partial t} + \nabla \cdot [\rho(x) \mathbf{v}(x,t)] = 0, \quad (3.58)
\]

\[
\rho(x) \frac{\partial \mathbf{v}(x,t)}{\partial t} = -\nabla \bar{\sigma}(x,t) + \nabla [\mu(x) \mathbf{u}(x,t)] + \rho \mathbf{f}, \quad (3.59)
\]

\[
\bar{\sigma}(x,t) = \frac{\kappa(x)}{\rho(x)} \delta \rho(x,t), \quad (3.60)
\]

where \(\bar{\sigma} = \frac{1}{2}(\sigma_{xx} + \sigma_{zz})\) is the average tensile stress and \(\kappa = \lambda + \mu\) is the bulk compression modulus. Here, an outline is given of the procedures of the lattice Boltzmann simulation. A square lattice with unit spacing is used on which each node has 8 nearest neighbors connected by 8 links (see Figure 3.7). Particles can only reside on the nodes and move to their nearest neighbors along these links in the unit time step. Hence, there are two types of moving particles. Particles of type I move along the axes with speed \(|e^I| = \nu_0\) and particles of type II move along the diagonal directions with speed \(|e^{II}| = \sqrt{2}\nu_0\) where \(\nu_0 = \frac{\lambda\nu}{\Delta t}\). Rest particles with speed zero are also allowed at each node. The occupations of the three types of particles are represented by the single-particle distribution, \(f_i^\sigma(x,t)\), where \(\sigma\) and \(i\) indicate the type of particle and the velocity direction, respectively. The distribution, \(f_i^\sigma(x,t)\), is proportional to the probability of finding a particle at node \(x\) and time \(t\) with velocity \(e_i^\sigma\). The particle distribution satisfies the following lattice Boltzmann equation:

\[
f_i^\sigma(x + e_i^\sigma \Delta t, t + \Delta t) - f_i^\sigma(x, t) = \Omega_i^\sigma, \quad (3.61)
\]

where \(\Omega_i^\sigma\) is the collision operator representing the rate of change of the particle distribution due to collisions. According to Bhatnagar, Gross and Krook (BGK) (Bhatnagar et al., 1964), the collision operator is simplified by the single time relaxation approximation. Hence, the lattice Boltzmann BGK equation is

\[
f_i^\sigma(x + e_i^\sigma \Delta t, t + \Delta t) - f_i^\sigma(x, t) = -\frac{1}{\tau} [f_i^\sigma(x, t) - f_i^\sigma^{eq}(x, t)], \quad (3.62)
\]
where \( f_i^{(eq)}(x, t) \) is the equilibrium distribution at \((x, t)\) and \( \tau \) is the single relaxation time which controls the rate of approach to equilibrium. The density per node, \( \rho \), and the macroscopic velocity, \( v \), are defined in terms of the particle distribution by

\[
m \sum_\sigma \sum_i f_i^\sigma = \rho, \tag{3.63}
\]

and

\[
m \sum_\sigma \sum_i f_i^\sigma e_i^\sigma = \rho v. \tag{3.64}
\]

where \( m \) is the particle unit mass. The equilibrium distribution can be chosen in the following form for particles of each type:

\[
f_0^{(eq)} = \alpha \frac{\rho}{m},
\]

\[
f_i^{(eq)} = \frac{1 - \alpha}{5} \frac{\rho}{m} + \frac{\rho}{3m} \frac{e_i^I \cdot V}{\nu_0^2},
\]

\[
f_i^{II(\text{eq})} = \frac{1 - \alpha}{20} \frac{\rho}{m} + \frac{\rho}{12m} \frac{e_i^{II} \cdot V}{\nu_0^2}, \tag{3.65}
\]

where the parameter \( \alpha \) is the fraction of particles with zero speed in equilibrium, and

\[
V = V(x, t) = v(x, t) + \frac{\tau(x)}{\rho(x, t)} \nabla [\mu(x) \nabla u(x, t - \Delta t)]. \tag{3.66}
\]

For sufficiently small particle velocity, \(|v| \ll \nu_0\), the resulting wave equation can be expressed in the form Equations (3.58) – (3.60) with the bulk compression modulus

\[
\kappa = \frac{3(1 - \alpha)}{5} \nu_0^2 \rho, \tag{3.67}
\]

and the shear modulus

\[
\mu = \frac{2(\tau - 1)}{6} \nu_0^2 \rho. \tag{3.68}
\]

The detailed derivation of the lattice Boltzmann model is similar to the one in the acoustic case given in Section 3.2. However, to be consistent with the lattice configuration of nine velocities, a nine-point template (Yanosik and McCracken, 1978) for displacement,

\[
\Delta u^E = \frac{1}{12} [u_{NE} - u_N + 10(u_E - u_K) + u_{SE} - u_S] \tag{3.69}
\]

was used to evaluate the derivative for the E-face. The component subscript has been omitted for clarity. Similar expressions may be written for the other three faces.
Having chosen the appropriate lattice size and the characteristic velocity for the lattice Boltzmann system, the shear modulus, \( \mu \), of the problem can be calculated for a given Re number and local density and then the relaxation time is determined by the formula above. Starting from an initial state of \( f_i^e(x, t) \), the density and velocity fields and hence the equilibrium distribution can be obtained. In each time step, the updating of the particle distribution can be split into two substeps: collision and streaming. It is irrelevant which one is the first for a long time run. The collision process at position \( x \) occurs according to the right hand side of the Boltzmann equation given as Equation (3.62). The resulting particle distribution at \( x \), which is the sum of the original distribution and the collision term, is then streamed to the nearest neighbor of \( x, x + \mathbf{e}_i \Delta t \), according to the particle velocity \( \mathbf{e}_i^e \). The updating procedure is terminated by attaining the required time period.

To impose the correct physical boundary conditions, let us consider the method proposed by Bayliss et al. (1986). Based on a one-dimensional analysis (i.e., neglecting the \( x \) derivative for the top boundary), the quantity

\[
R_1 = \sqrt{\rho \mu u_x + \sigma_{xz}} \tag{3.70}
\]

is converted toward the boundary with velocity \( u_s \),

\[
R_2 = \sqrt{(\lambda + \mu)\rho u_z + \sigma_{zz}} \tag{3.71}
\]

is converted toward the boundary with velocity \( u_p \) and

\[
R_3 = (\lambda + \mu)\sigma_{xx} - \mu \sigma_{zz} \tag{3.72}
\]

moves with zero velocity. We specify \( R_1 \), \( R_2 \) and \( R_3 \) by the values extrapolated from the interior nodes. This, combined with the free surface conditions (\( \sigma_{zz} = \sigma_{xz} = 0 \)), enables us to value the average tensile stress \( \bar{\sigma} \). Following the same procedure as in acoustic case, let \( f_i^{e(IN)} \) denote the incoming particle distribution along \( \mathbf{e}_i^e \) and \( f_i^{e(OUT)} \) the outgoing particle distribution along \(-\mathbf{e}_i^e\). Using Equation (3.65) we have the following relation,

\[
f_i^{f(IN)} = \frac{2(1 - \alpha) \rho_0}{m} \left( \frac{1 - \bar{\sigma}}{\kappa} \right) - f_i^{f(OUT)},
\]

\[
f_i^{\Pi(IN)} = \frac{1 - \alpha \rho_0}{10} \left( \frac{1 - \bar{\sigma}}{\kappa} \right) - f_i^{\Pi(OUT)}. \tag{3.73}
\]

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In addition to the free surface, there are three other boundaries. These are all artificial boundaries and appropriate absorbing boundary condition must be imposed. We use the one-dimensional characteristics given by the above equations (or the analog one obtained by neglecting z derivatives when the boundary is the line x=constant) and impose the boundary condition that the incoming characteristic variable is zero. These conditions are exact for compressional and shear waves impinging normally on the boundary. Since they are based on one-dimensional characteristics, they do not absorb Rayleigh waves. The Rayleigh wave reflection will be ameliorated by further use of a simple spatial filter, or sponge to their time marching solution that gradually diminishes the amplitude of the wavefield toward the artificial boundaries (Israeli and Orszag, 1981; Dai et al., 1994). However, the damping coefficient is experimentally determined and is usually small. In all the following simulations the coefficient is set to 0.025.

3.3.2 Numerical examples

Source excitation There are numerous ways of initiating the forward modeling. In this work, we consider three types of sources, namely, a localized directional body force, a pressure source, and a shear source. For the directional force, $f^F_x(i,j)$ (or $f^P_x(i,j)$) is introduced at site (i,j) at $n^{th}$ step over a small region of the grid. In the calculations, we have used a Gaussian distribution for the force given by

$$f^F_x(i,j) = h^n \exp\{-\alpha^2[(i - i_0)^2 + (j - j_0)^2]\}. \quad (3.74)$$

where $i_0$ and $j_0$ give the center of the force, $h^n$ gives its time history, and $\alpha$ determines the degree of concentration. In most calculations, we have chosen $\alpha = 1$ which gives rapid decay. For the pressure source, $f^P_x(i,j)$ and $f^S_x(i,j)$ are derived from a scalar potential $\phi^n(i,j)$ by differentiation

$$f^P_x(i,j) = \frac{\partial \phi^n}{\partial x}(i,j) \quad (3.75)$$

and

$$f^S_x(i,j) = \frac{\partial \phi^n}{\partial z}(i,j). \quad (3.76)$$

The set of body forces derived from $\phi^n$ generate only P waves (Aki and Richards,
1980) and therefore comprise a pressure source in distinction to a shear source. For the spatial distribution, we have chosen a relation as in equation (3.74).

For the shear source, we derive \( f_x^n(i, j) \) and \( f_z^n(i, j) \) by taking the curl of the potential
\[
f_x^n(i, j) = \frac{\partial \psi^n}{\partial z}(i, j) \tag{3.77}
\]
and
\[
f_z^n(i, j) = \frac{\partial \psi^n}{\partial x}(i, j), \tag{3.78}
\]
where the spatial distribution is again given by Equation (3.74).

**Accuracy evaluations** First we consider elastic wave propagation in an elastic full space. The P-wave and S-wave velocities were chosen to be 3000 m/s and 1732 m/s, respectively, which correspond to a Poisson ratio of 0.25. The source has a Ricker-like time history with a dominant frequency of 50 Hz. The source acted as a point force in the vertical direction and was located at the center of the numerical grid. Figures 3.8 and 3.9 show comparisons of analytical and numerical seismograms, for single traces in both horizontal and vertical velocities, respectively. The height of the receivers above the source was 50 m. The horizontal distances between the source and the receivers were 50 m, 125 m and 200 m, respectively. There is a good agreement of the analytical and numerical solutions, although the numerical wave has a slightly lower amplitude than does the analytical wave when the wave propagates far from the source. This slight misfit is caused by numerical dispersion.

Next we consider elastic wave propagation in a medium containing two half-spaces with different material parameters which are in contact. The upper region has P-wave and S-wave velocities of 2000 m/s and 1153 m/s, respectively. Lower region P-wave and S-wave velocities are 3000 m/s and 1732 m/s, respectively. The configuration of the modeling problem is shown in Figure 3.10. The uniform density was chosen to be equal to unity. A point pressure source was embedded in the medium with the low velocity, at a height of 50 m above the interface. The horizontal distances between the source and the receivers were 75 m and 100 m, respectively. The Ricker wavelet source has a peak frequency of 20 Hz. The calculations used a grid size of 500 X 500, which corresponds to a model size of 800 X 800 m². Absorbing exterior boundaries were used. Figures 3.11 and 3.12 show the results of the lattice Boltzmann method in
Figure 3.8: Comparison between numerical (dashed) and analytical (solid) horizontal components for a full-space at three different stations.
Figure 3.9: Comparison between numerical (dashed) and analytical (solid) vertical components for a full-space at three different stations.
Figure 3.10: Location of receivers for numerical and analytical comparisons for a horizontal interface model.

The results are in good agreement and only small differences are observed.

Figure 3.13 represents the corner model used in this numerical example. It consists of two media with a high velocity inside the corner. The corner has P and S-wave velocities of 1732 and 1000 m/s, respectively, the P and S-wave velocities of the outer region are 1154 and 666 m/s, respectively. A grid size of 384 X 200 was employed. The grid space of horizontal and vertical components was 1.825 m. The source is a point pressure centered at grid (110, 61). The force time source is the Ricker wavelet with dominant frequency of 50 Hz. A time interval of 0.75 msec was used.

As an aid to visualization of the propagation of elastic waves in the presence of the 90 degree corner, a series of time “snapshots” of vertical and horizontal components of displacement at a given instant and at all ranges and depths computed are displayed in Figures 3.14 and 3.15, respectively. In the first snapshot, the direct P-wave from the line source appears with a cylindrical wavefront. P-waves, S-waves, head waves,
Figure 3.11: Comparison between numerical (dashed) and analytical (solid) horizontal components for a horizontal interface model at two different stations.
Figure 3.12: Comparison between numerical (dashed) and analytical (solid) vertical components for a horizontal interface model at two different stations.
and diffracted waves appear in the final snapshot. The intervening snapshots illustrate the increasing complexity of the interaction of the original P-wave with the 90 degree corner and with the edges of the model. In the first snapshot, at a traveltime $t = 94$ ms (Figures 3.14(a) and 3.15(a)), a single P-wave appears with upward first motion above the source and downward first motion below the source. At this time the wavefront has just reached the layer interface below the source. The direct P-wave has reached the free surface in the snapshot at $t = 132$ ms (Figures 3.14(b) and 3.15(b)). Reflected and refracted waves have been produced by the P-wave which strikes the interface below the source. At $t = 170$ ms, Figures 3.14(c) and 3.15(c) show the direct P-wave reflected from the free surface. For the first time, the S-wave, refracted into the quarter-space, can be distinguished from the P-wave. Since the PS-wave diffraction has significant vertical motion when propagating horizontally, it is easily visible on the snapshot of vertical motion. The PP-wave, diffracted from the corner, on the other hand, is easily distinguished on the snapshot of horizontal motion since its motion is principally horizontal. The head wave generated by the P-wave which refracts into
Figure 3.14: The horizontal component of seismograms for the corner-edge medium at times 94(a), 132(b), 170(c), 208(d) and 246(e) ms, respectively.
Figure 3.15: The vertical component of seismograms for the corner-edge medium at times 94(a), 132(b), 170(c), 208(d) and 246(e) ms, respectively.
the high-velocity quarter-space and back into the low-velocity half-space exhibits a plane wavefront. This front connects the refracted P-wave event with the reflected P-wave event, in accordance with theoretical expectations. The PS-reflection from the layer is visible for the first time in the snapshot at $t = 208$ ms (Figures 3.14(d) and 3.15(d)). The PS-head wave is also visible as a plane wavefront intersection in both the diffracted PS-wave and the refracted P-wave events. The P-wave and S-wave reflections from the free surface separate in the snapshot at 246 ms (Figures 3.14(e) and 3.15(e)). Various wavefronts including the direct wave, the diffraction, reflected-converted, and transmitted fronts, are seen clearly in the final snapshots, where the reflections from model boundaries are efficiently absorbed.

3.3.3 Summary

We have shown that elastic wave propagation can be simulated by a lattice Boltzmann method. The scheme presented here permits an accurate and robust implementation of both the free surface condition and the absorbing boundary condition.

The main limitations of the lattice Boltzmann method come from the numerical dispersion and the finite numerical size of the grid. With these restrictions, interpretation of numerical seismograms may be very difficult for complex media. In order to increase accuracy, it would be desirable to develop a high-order lattice Boltzmann scheme. It must be pointed out that in all the numerical examples above, the computation of the displacements is simply a summation of particle velocities. Use of a better integration formula could improve the results.
Chapter 4

Applications of Microscopic Simulations in Porous Media

4.1 Rock Pore Geometry

Porous media are aggregates of solid elements (grains, matrices, etc.) between which the voids form the pore space itself. These voids within the porous media give rise to the wide differences in physical behavior between dense solids (such as minerals) and porous substances, which are complicated assemblages in which the presence of a fluid, even in very small amounts, adds to the overall complexity. To stress the importance of the physical properties of rocks as input in many geophysical methods, Archie (1950) devised a new term, petrophysics, to designate the area of geophysics dedicated to measuring and modelling the physical properties of rocks. In the same paper, Archie pointed out that meaningful petrophysical models must be based on knowledge of the microstructure of the rocks. However, the complexity of reservoir rocks is clearly too great to be incorporated with all its details in petrophysical models. Instead, extensive simplifications are usually made. Considering the transport properties of rocks, for example, the most common approach is to assume a pore geometry model (i.e., an idealized representation of the pore space in which the flow equations can be solved). Pore geometry models are quantitatively summarised by discrete sets of parameters such as porosity, shape and size parameters, connective tortuosity, and so forth (Scheidegger, 1974; Dullien, 1979).
4.1.1 Modeling of porous media

Modeling of porous media has been done recently in an effort to learn more about how the rock, pore space, and fluids control the rock properties measured and to interpret better those measurements made in the field and laboratory. Over the years, many models of porous media have been developed, most of which have been motivated by a certain phenomenon, and often the model could be used to study that particular phenomenon and predict some of its properties. However, these models were not general enough to be useful for studying other problems, and they often contained parameters that either were defined very vaguely or had no physical meaning whatsoever, and their sole purpose was to make the models’ predictions agree with experimental data. The problem is that each model has a different representation of the “pore space/grain space” of the rock and many models have contradictory or unrealistic representations. Transport models require a fully-connected pore space to calculate the transport of fluid and electricity across the rock. Yet most velocity models represent the pore space as nonconnected inclusions, with the scattering theory models requiring the pores to be more than one pore width apart. In Sen et al.’s (1981) electrical model, spheres of nonconducting material are imbedded in a conducting material until the desired concentration is reached. However, the reverse (conducting spheres in a nonconducting medium) never allows for a conducting path.

Two exciting areas of porous media modeling today are the calculation of rock properties from direct observation of the pore space and the simultaneous modeling of several different rock properties for better understanding of the relationships between properties. Research in the first area was done by Dullien (1979), Lin and Cohen (1982), Wilkens et al. (1984), and Ehrlich et al. (1991). The Lin and Cohen (1982) model is a computer representation of a rock built from SEM image analysis of many serial thin sections. Their model mispredicted the measured permeability of the rock by an order of magnitude but predicted the formation factor within a factor of two and the porosity to within 5 percent. Dullien’s (1979) model calculated bivariate pore size distributions from thin section and mercury injection and predicted the permeability and formation factor of over twenty sandstones quite well. Wilkens et al (1984) were able to predict velocities to within 5 percent using a trimodal distribution of aspect ratios. Ehrlich et al. (1991) devised a fast image analysis technique which produces
over 100 pore parameters which can then be correlated with petrophysical properties.

Despite the fact that each model has a different representation of the pore space for different properties, a single realization of the pore space/grain space controls all the physical properties of a particular rock. By modeling a variety of properties with a single model, the model becomes more contained and unique, thus promoting better understanding of the relationships between the properties. One most promising of such models is based on a fractal concept (Mandelbrot, 1982).

4.1.2 Fractals and porous media

The concept of fractals, introduced by Mandelbrot (1982), has proven to be a highly useful way to describe the statistics of naturally-occurring geometries. Fractals enter the problem of fluid transport in porous medium in at least two distinct ways. First, the fractal pore-structure information might be used directly to calculate the permeability of porous rock. Second, the paths formed by flowing fluids or ions in pores may be described by fractal models such as result from percolation theory, or the path of the underlying pore geometry.

Adler and coworkers (Adler 1989) have pioneered the development of permeability models on well-defined, deterministic fractal structures. Stokes equations are solved for one- to three-dimensional geometries of single or multifractal character. The systematics developed may help establish ties between the geometric concept of the fractal dimension of the pores and transport properties like permeability. Such connections between geometry and transport might be generalized to more complicated or statistical fractal structures. Grain and pore sizes for rocks frequently follow a log-normal distribution. However, it has been observed that many rocks have a fractal distribution of features at small scales (less that approximately one hundred microns). Our work here is aimed at generating fractal networks having the statistics of rock-pore systems. Before doing so, let us introduce the definition of a fractal distribution. If the number of objects \( N_i \) with a characteristic linear dimension \( r_i \) satisfies the relation

\[
N_i = \frac{C}{r_i^D},
\]

a fractal distribution is defined with \( D \) the fractal dimension and \( C \) a constant of a fractal proportionality. Fractal concepts can also be applied to a statistical distribution
Figure 4.1: A typical rock structure generated by a fractal generator with prescribed dimension and porosity. The black regions represent the grain material.

of objects. Such is the case if the number of objects $N$ with a characteristic linear dimension greater than $r$ satisfies the relation,

$$N = \frac{C}{r^D}. \quad (4.2)$$

Mathematical representations (4.1) or (4.2) can be valid over an infinite range. However, for any physical application there will be upper and lower limits on the applicability of the fractal distribution. The essential feature of the fractal distribution is its scale invariance. No characteristic length scale enters into the definitions (4.1) or (4.2). If scale invariance extends over a sufficient range of length scales then the fractal distribution provides a useful description of the applicable statistical distribution. The fractal dimension $D$ provides a measure of the relative importance of large versus small objects.

We now describe a procedure to create 2-D fractal porous structures. The basic concept is to distribute features of microgeometric pore space randomly in a region, using an appropriate number density function. In a fractal medium, the number
density $m$ of features of size $L$ is given by

$$m(L) = AL^{2-D},$$

(4.3)

where $D$ is the fractal dimension and $A$ is a coefficient which depends on the material. The following procedure may be used:

1. Pick a set of feature sizes. The sizes must lie in the range of validity of a fractal model. Typically, each successive size is picked by dividing the previous size by a factor of two.

2. Determine the number density for each feature size using Equation (4.3). Calculate $\Delta = \Delta x = \Delta y = 1/m(L)$. Divide the region of interest into subdomains of size $N\Delta x, N\Delta y$, where the value of $N$ is supplied by the user. The overall dimensions of the region must be whole multiples of $N\Delta$. The expected number, $E(L)$, of feature size $L$ in each subdomain is $N^2$.

3. Within the specified subdomains, the expected number of features of size $L$ are distributed randomly. Feature shapes can be chosen as square and circles. The largest feature is distributed first. Smaller features can overlap the large ones previously distributed. We restrict the locations of features to the subdomains. This restricts the possible realization, mainly by eliminating those realizations with extreme variations due to large scale clumping of features. The structure obtained should be characteristic of the material to be described. The values of $N\Delta x$ and $N\Delta y$ are usually considerably larger than the corresponding $L$, so the restriction to placement within a subdomain is not a strong one.

4. The nature of any feature, i.e., whether it represents a solid grain or an open region, is determined probabilistically. Initially, all lattice sites are set to "grain" and an input quantity $b$, ranging between 0 and 1, is used to control the final porosity. A feature is declared a grain if

$$\text{Min}(1, \text{int}(\text{rand}/b)) = 1,$$

(4.4)

otherwise, it represents open space. In Equation (4.4), 'Min' is the minimum operation, 'rand' is a random number between 0 and 1, and 'int' is the greatest integer function. This procedure produces a structure with porosity close to $b$. 
We generated the porous structure shown in Figure 4.1 using a feature size spectrum of \((32, 17, 10, 5, \ldots)\), given in terms of number of lattice sites, a fractal dimension of 2.5, and the factor \(A = 0.12\). Total porosity of the sample was calculated to be 0.42.

4.2 Calculations of Rock Permeability

There have been numerous theoretical and experimental studies attempting to predict permeability from known rock properties. These investigations are diverse in approach, but they may be classified broadly into three categories based on their use of microscopic data, as we mentioned earlier. First, some studies employ no microscopic data at all; these studies attempt instead to relate permeability to other, more easily measured, macroscopic rock properties such as resistivity and porosity. In the second category are studies that collect microscopic data on pore-space geometry, usually via microscopy and digital image analysis, and then compute macroscopic statistics from these microscopic data in an attempt to relate permeability to the statistical properties. The third class of investigations is based entirely on microscopic rock geometry. The challenge in this final category is to develop a numerical model for fluid flow capable of reproducing enough of the physics of real fluids in real porous media that permeability can be predicted accurately. However, because of the very complicated boundaries in pore structure, a macroscopic framework cannot provide exact solutions of flow through porous media and diffusion in pores. Lattice gas methods have been shown to have the capability of solving these problems (Rothman, 1988; Succi et al., 1989). The key difference between cellular automaton models and existing theoretical literature on permeability lies in the numerical method used to model fluid flow. Previous numerical techniques have typically employed arrays of geometrically simple pores, throats, and cracks; the results have been approximate models of microscopic flow. The utility of cellular-automaton fluids for computations of porous flow stems from the ease with which computations are made in grossly irregular geometries; no special grids are required, and the appropriate boundary conditions are easily applied at all solid-fluid boundaries.

The objective of this section is to test lattice gas flow past complicated boundaries and to verify that this method reproduces Darcy's law for low Reynolds number flows.
through porous media. We present some quantitative results and estimate the utility of the lattice gas model. Permeability as a function of fractal dimension and porosity are also presented. At the end of this section we will describe a two-phase immiscible lattice-gas model and demonstrate phase separation due to surface tension.

4.2.1 Lattice-gas model

Cellular automaton fluids evolve in time according to extraordinarily simple rules. The basic idea is to construct a lattice gas. Figure 4.2 shows the original FHP model (Frisch et al., 1986), which will be described here. To simulate a fluid in equilibrium, particles initially populate the lattice at random locations. Each particle has unit mass and moves with unit speed in one of the six possible directions. The possible velocities correspond to the six links on the triangular lattice and are given by the unit vectors $c_i$ through $c_6$, where

$$ c = \left\{ \cos \left[ \frac{2\pi i}{6} \right], \sin \left[ \frac{2\pi i}{6} \right] \right\}, \quad i = 1, \ldots, 6. $$

(4.5)
At each site on the lattice, only one particle can move in each direction, but up to six particles can populate any one site. Evolution proceeds in discrete time steps via a two-step process. In the first, the particles move one unit along one of the hexagonal paths. In the second, the existence of a collision is identified. If no collision occurs, the particles go on to the next time step with their direction of travel unchanged. If a collision occurs, all particles involved in the collision have their directions of travel deflected by 60°. In Figure 4.2, the first or “move” part of the cycle is represented by “a”. The second part of the cycle is represented by two parts: collision identification in “b” and the response in “c”. This process is repeated at each subsequent time step.

The non-slip condition at boundaries is easily implemented by reversing the velocity of the particles which hit the boundaries. There are two ways to create a pressure gradient between the planes x=0 and x=L. The first one, we will use here, is to use a uniform forcing condition at the inlet. There, we can use a prescribed uniform flipping rate, which produces a net momentum increment in the flow direction. Because the pressure change is linearly proportional to the forcing rate, the pressure change can be prescribed. Another method is to maintain a high pressure at the inlet and low pressure at the outlet by using different densities. Because the pressure is linearly proportional to density for small velocities, we have a pressure drop between x=0 and x=L. Simulations show an equivalence between these two methods for channel flow. Statistical methods are also used to obtain macroscopic quantities. A time average or spatial average is required. We are interested in the detailed flow structure for arbitrarily complicated boundaries and the calculation of permeability using steady state measurements, so we use a time average for steady flows to reduce the microscopic noise.

It should be pointed out that the algorithm described above or its variations have been used by various authors to investigate flow phenomena in porous media. We paid special attention to the efficient implementation of simulations. Riccardi, Bauer and Lim (1991) presented a vectorized supercomputer implementation of a cellular automaton model for lattice-gas hydrodynamics. Using a 32-bit “C” compiler, we have written a similar vectorized algorithm of a cellular automaton model in porous media, which is executed on a 33-MHz 80486-based computer system with, of course, only a single processor. It contains a built-in lookup-table-based algorithm which
does temporal and spatial bit-level averaging ten times faster than the conventional approach. Interestingly, a non-vectorized algorithm for the numerical simulation of hydrodynamics with lattice-gas automata in two dimensions (d'Humieres and Lallemand, 1987) implemented on a floating-point array processor (FPS-164) is 50% slower than our desktop emulator! (Since cellular automata do not use floating-point arithmetic, a floating-point array processor becomes wasted hardware.) However, the raw speed of a supercomputer cannot be dismissed. Riccardi et al. ran their algorithm on a single processor of an ETA10-G vector supercomputer with a performance of 37.99 million node-updates per second. By comparison, our version of their algorithm coded for our 80486-based system performed 0.788 million node-updates per second, which is slower by a factor of 48.2. For the lattice-gas simulation in porous media, Rothman’s (1988) computations were performed on a Sun 3/160 workstation and yielded a performance factor of 0.078 million node-updates per second while the performance factor in our case was 0.208 million node-updates per second, which is 3.6 times faster. Since the Sun workstation is faster than our 80486-based system, our better performance factor is a direct consequence of our more-efficient software.

4.2.2 Numerical experiments

An elementary example of fluid flow that satisfies Darcy’s law is the plane Poiseuile flow between two parallel plates, illustrated in Figure 4.3. Because parallel-plate flow is a simple model for flow through a crack or joint of a rock, it is the object of extensive study (see, for example, Brown, 1987). In Figure 4.3, only two dimensions are shown: flow is assumed to be invariant along the third dimension. If the pressure gradient along this 2-D channel is uniform, then the velocity u of the fluid will be everywhere parallel to the channel walls. Thus, for the coordinate system shown, \( u_x = 0 \). The \( x \) component of velocity is strongly influenced by the interaction of the fluid with the walls of the channel. In fluid mechanics in general and porous flow in particular, the velocity of viscous fluids at solid boundaries is usually assumed to be zero; this is the "no-slip" boundary condition. Frictional (viscous) forces then dictate that the flow through the channel be fastest in the centre, the position farthest from the walls. The precise velocity profile is easy to derive (see, for example, Tritton, 1977) and is given
Figure 4.3: The geometry of 2-D channel flow. Flow is invariant in the third dimension and may be taken to be between two parallel plates. The velocity $u$ of the fluid vanishes at the boundary. A uniform pressure gradient in the $x$-direction produces a parabolic velocity profile.

by the parabolic relation

$$u_x = \frac{G}{2\mu} \left( \frac{d^2}{4} - y^2 \right), \quad (4.6)$$

where the pressure gradient, $G = -dp/dx$, $\mu$ is the viscosity, and $d$ is the distance between the two plates. To find the volumetric rate of flow per unit area $q$, integrate $u_x$ from $y = -d/2$ to $y = d/2$ and divide by $d$, to obtain

$$q = \frac{Gd^2}{12\mu}. \quad (4.7)$$

Comparing Equation 4.7 with Equation 4.6, we find the well-known result that the permeability of two parallel plates separated by a distance $d$ is $k = d^2/12$. Numerical data are obtained by doing time averages (over 5000 time steps) which are shown in Figure 4.4. Good matches between theory and numerical data verify the method and the program used.

Using lattice gas simulations, we have studied the relationship between permeability, porosity and fractal dimension. Several simulations have been performed. The medium is generated with given porosity and fractal dimension in a square two-dimensional region. For all calculations, we use nonslip conditions at the boundaries
Figure 4.4: Averaged velocity distribution. The solid line is the parabolic curve from the analytical solution and the squares indicate simulation results.

Figure 4.5: A typical lattice gas velocity vector field for a two-dimensional flow. The black regions represent the impermeable material.
Figure 4.6: Permeability (lattice units) versus porosity for fixed fractal dimension, $D=2.5$.

Figure 4.7: Permeability (lattice units) versus fractal dimension for fixed porosity, $\phi = 0.4$. 

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and the net flow is in the x direction. We present the relation between the permeability and porosity in Figure 4.6. As expected, an increase of porosity provides a monotonic increase in permeability. Figure 4.7 presents the relation between permeability and fractal dimension holding porosity constant.

4.2.3 Immiscible fluids

Two-phase immiscible fluids can be simulated by an extension of the original FHP-type lattice gas model. The important property to model two-phase flows is the surface tension between the fluids and the wettability between fluid and solid materials. Rothman and Keller (1988) were the first to extend the single-phase FHP (Frisch et al., 1986) lattice gas model to simulate multi-phase fluid problems. They introduced colored particles to distinguish between phases. A nearest-neighbor particle interaction was used to implement interfacial dynamics, such as Laplace's formula for surface tension. Later, Somers and Rem (1991) and Chen, S. et al., (1991c) extended the original colored-particle scheme by introducing colored holes. It has been shown (Chen, S. et al., 1991c) that the colored-hole lattice gas method extends the original nearest neighbor particle interactions to several lattice lengths, leading to a Yukawa potential. Moreover, the colored-hole scheme carries purely local information in its particle collision step, reducing the size of the look-up table in the algorithm and consequently speeding up the simulation. In the following we will describe this model.

The FHP hexagonal lattice was used as the basis of the model. As many as six moving particles and one rest particle with unit mass may occupy each lattice site simultaneously. All particles and holes are colored red or blue to distinguish the two fluids. For each direction at a given site, we assign a two-bit Boolean variable \((f_i(x,t), N_i(x,t))\), \(i = 0, 1, \ldots, 6\), for space \(x\) and time \(t\), where \(N_i = 1\) represents a particle and \(N_i = 0\) a hole; \(f_i = 1\) represents red and \(f_i = 0\) represents blue. This lattice-gas model requires 14 bits per site. Exclusion rules apply to particles and holes; therefore a particle and a hole cannot occupy the same state. As usual, the lattice-gas automata have two operations for each time step: streaming and collision. During the streaming process, particles or holes with \((f_i, N_i)\) move to their nearest-neighbor site, without change of color, along \(e_i, i = 1, 2, \ldots, 6\), the unit velocity in the \(i^{th}\) direction. Rest particles or rest holes stay at the original site. Let \((f, N)\) be the
initial state before a collision at site $x$ and time $t$, where $f = (f_0, f_1, \ldots, f_6)$ and $N = (N_0, N_1, \ldots, N_6)$. Define $(f', N')$ to be the output state after a local collision. Then, in order to ensure that the two-phase fluids satisfy the Navier-Stokes equation, we require the conservation of particle number for each color and the conservation of total momentum during the collision processes:

\[
\sum_i N_i f_i = \sum_i N'_i f'_i,
\]
\[
\sum_i N_i (1 - f_i) = \sum_i N'_i (1 - f'_i),
\]
\[
\sum_i N_i e_i = \sum_i N'_i e_i.
\]  

(4.8)

For single-phase cells, where particles of one color occupy the cell, Equation (4.8) will become the same constraint as that of FHP models (Frisch et al., 1987). Therefore each single phase still satisfies the Navier-Stokes equations.

The essential idea in these collision rules is to have the color holes act as the memory of the same color particles and to let this color information propagate by the streaming of holes. Colored particles move in the opposite direction of the colored-hole flux when collisions occur. Therefore, the color-hole field near a color interface plays an important role in determining the directions of colored particles after collisions. Colored holes are created and destroyed as follows: When a particle changes direction in a collision, a hole of the same color is created in the original direction. A particle annihilates any hole if one exists in the new direction. Thus, the consequence of this rule for colored holes is that information about the local particle color is transmitted by the holes a distance on the order of a mean free path.

In the FHP model (Frisch et al., 1986), collisions only occur when the particles meet at the same lattice site at the same time. Therefore the FHP-type collision is equivalent to scattering between particles interacting with a hard core with zero radius. The simulation of surface tension in two-phase fluids required short-range attractive potentials between identical particles. To incorporate this attractive force, we let the particle collisions depend on the local color fields. We introduce a local flux for the colored particles, $G$, and a local flux for the colored holes, $F$, as follows:

\[
G = \sum_i (2f_i - 1) N_i e_i.
\]

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\[ F = \sum_i (2f_i - 1)(1 - N_i)\mathbf{e}_i. \]  \hspace{1cm} (4.9)

The rules for particle collisions are as follows:

(i) Choose the output state to maximize the quantity \( Q = -\mathbf{F} \cdot \mathbf{G}' \), where \( \mathbf{F} \) is calculated from the given input hole state before a collision and \( \mathbf{G}' \) is calculated for the output particle state. This constant ensures that the colored particles move in the direction opposite the local color-hole flux.

(ii) If there are several configurations, \( \mathbf{G}' \), which have the same maximum value of \( Q \), we choose the output having the minimum \( |\mathbf{G}'| \). This step directs the colored particles as closely as possible in the opposite direction of the local color-hole flux and stabilizes the plane interface and the circular interface.

(iii) If there are still several possible configurations, then we choose the output state with a rest-particle. This slows the flow of the fluid and enhances phase separation.

(iv) If there are still several configurations, then we choose the output that will minimize the viscosity. This step usually requires that the output state be different from the input state.

(v) If the above steps do not give a unique output state, we randomly pick one of these states.

With this procedure, the FHP collision-saturated rules (Diemer et al., 1989) (modified to preferentially enhance the rest particle state) are automatically recovered in a single-phase region.

A C program based on this scheme has been implemented on IBM/PC computers. Because the rules are purely local, a table-look-up algorithm is developed for \( 2^{14} = 16384 \) configurations. In Figure 4.8 we show frame-buffer displays for two-phase separation. The system has 256 X 256 lattice sites with periodic boundary conditions. The initial particle and hole color configuration is randomly distributed and the density, \( d \), is 0.4 particles per direction. The ratio of red particles to blue particles, \( d_r/d_b \), is unity, where \( d_r \) and \( d_b \) are the red particles per state and blue particles per state, respectively. Identically colored particles cluster because of the interaction potentials. Because of the Brownian motion of the color drops, the color drops gradually merge and form bigger drops. The final stable state is the minimum surface energy state, which has an energy proportional to the length of the interface. We see that at time 45000 all red and blue particles have separated, forming a stable
Figure 4.8: Nonequilibrium evolution of an immiscible, two-fluid, hexagonal-lattice automaton at time steps $t = 0, 400, 3600, \text{ and } 40,000$. The initial configuration (top left, $t=0$) is a random mixture. In the final state (bottom right, $t = 40,000$), the two fluids have separated due to surface tension. The system has $256 \times 256$ lattice sites with periodic boundary conditions. The total fluid-density is 0.4 with a red-to-blue particle ratio equal to unity.
Although the two-phase lattice gas algorithms described are able to produce interesting surface phenomena, they are difficult to compare quantitatively with experiments and other numerical simulations due to noise induced by particle fluctuations. Combining the lattice Boltzmann ideology with their original idea of using particle-particle nearest neighbor interactions, Gunstensen et al. (1991) first proposed a lattice Boltzmann method for solving two-phase fluid flows. An important contribution of this model is the explicit introduction of a perturbation step so that Laplace's formula at an interface can be approximated. Recently, Grunau et al. (1993) have extended this model by including density and viscosity variations. These models have been used for simulating fluid flows in porous media for understanding fundamental physics related to enhanced oil recovery and predicting the relative permeability (Rothman, 1990; Gunstensen and Rothman, 1993). Simulation results compare well with experimental measurements of flow patterns and relative permeability (Grunau, 1993).

4.3 Wave Propagation in Porous Media

In this section we study wave propagation in porous/crack media using a lattice Boltzmann method. The particle interpretation of lattice Boltzmann method allows the use of very simple boundary conditions even for complex geometries. This permits flexible, fine-scale positioning of the grain and pore boundaries. A primary goal was the study of the scattering of seismic waves by cracks in the porous medium of propagation which causes a diminution of the wavefront's energy. We study this effect, known as apparent attenuation, in several simulated porous media. This attempt has never been made, to the best of our knowledge. The investigation process is straightforward: 2-D porous media with imposed porosity and fractal dimension are generated by the fractal generation method described in Section 4.1 and the wave equation is solved by the acoustic lattice Boltzmann method described in Section 3.2. Solving the wave equation directly is advantageous from the standpoint of mathematics, since it is free of any additional assumptions that would otherwise be required.
4.3.1 Example of seismic wave attenuation

Macroscopic attenuation of seismic waves in porous media and rocks can be explained microscopically. To see this, let us consider a medium in which the porosity consists of spherical cavities of radius $r$, isolated from each other (Figure 4.9).

Let us now assume that an incident P wave propagates into this medium. The P and S-wave velocities of the medium corresponding to the supposedly elastic matrix are denoted $v_p$ and $v_s$. The incident wave is expressed by

$$u_z = u_{z0} \exp [i(kz - \omega t)], \quad (4.10)$$

where $kv_p = \omega$, the incident energy per unit area being written

$$e_0 = \sigma_{xx} \frac{\partial u_x}{\partial t}. \quad (4.11)$$

Stress $\sigma_{xx}$ is determined from (4.10) by

$$\sigma_{xx} = (\lambda + 2\mu) \frac{\partial u_x}{\partial x}, \quad (4.12)$$
where $\lambda$ and $\mu$ are the Lamé constants (see Chapter 3). The average incident energy over a period, defined by

$$e_0^{av} = \frac{\omega}{2\pi} \int_0^{2\pi} e_0 dt$$

(4.13)

can be written from (4.10), (4.11) and (4.12) as

$$e_0^{av} = -\frac{1}{2}(\lambda + 2\mu)\omega k u_2^2.$$  

(4.14)

When the incident wave meets a spherical cavity, an elementary scattering process occurs. The scattered wave is the superposition of two waves, an S wave and a P wave. This scattered wave radiates energy in all directions, and the energy is subtracted from the incident wave energy. The latter is accordingly attenuated. To quantify the elementary scattered energy, it is customary to introduce the notion of scattering cross-section $S_E$ which is the ratio of the average energy scattered over a period to the average incident energy per unit area. Hence, it has the dimensions of an area per unit time. If the cavities are sufficiently distant from each other, i.e. if the number of cavities $\bar{n}$ per unit volume is small (in practice, if the porosity is lower than 20%), it may be assumed that no interactions occur between the scattered waves (no interference, and no multiscattering effects). The scattering cross-sections can then be added (Waterman and Truell, 1961). This additivity of scattering cross-sections allows the approximation to the first order of multiple scattering to be made (Ishimaru, 1978). In this approximation, it is considered that the direct wave is no longer the incident wave defined by (4.10), but a wave attenuated by the elementary scatters on the path already travelled. More specifically, consider a direct wave of average energy per unit area. By definition of the scattering cross-sections and from the principle of their additivity, we have

$$e^{av} = e_0^{av} \exp(-2\alpha z), \quad u_x = u_{z0} \exp(-\alpha z) \exp[i(kx - \omega t)]$$

(4.15)

where attenuation $\alpha$ is

$$\alpha = \frac{1}{2} \bar{n} S_E.$$  

(4.16)

Theoretical studies are abundant in the area of apparent attenuation (Wu, 1982; Frankel and Clayton, 1986). However, instead of treating the energy decay of the wave front, the authors focus on the intensity decay of a plane harmonic wave. The
intensity $I^{av}$ decreases as

$$I^{av} = I_0^{av} \exp \left(-\frac{k \tau}{Q}\right),$$

(4.17)

where $Q$ is called the quality factor. Comparing (4.17) with (4.15), we have

$$Q^{-1} = \frac{\check{\eta} S_E}{k}.$$  

(4.18)

Many authors have investigated scattering effects by inclusions. Ying and Truell (1956), in particular, determined an expression for the scattering from spherical cavity inclusions. If the incident wavelength is large in comparison with the cavity radius $r$, or more precisely,

$$kr < 0.1,$$

(4.19)

they found

$$Q^{-1} = \phi g k^3 r^3,$$

(4.20)

where $\phi$ is the porosity and $g$ is a frequency independent constant. Equation (4.20) shows that $Q^{-1}$ is proportional to the cube of the frequency, and also to the cube of the cavity radius. Hence, scattering processes only become important at the very high frequencies.

### 4.3.2 Experimental procedure

Two-dimensional porous media can be generated by the fractal method with given porosity and fractal dimension. The wave propagation is computed by the use of lattice Boltzmann method. It is characterized by a mesh spacing $\Delta x$, which is carefully chosen in order to avoid numerical dispersion. The algorithms are fully discussed in Section 3.2. To model wave propagation in porous media, however, the boundary conditions between matrix and pores must be specified. A simple rule of Equation (3.36) was used at these boundaries to model a free surface boundary.

The simplest method to measure $I(r)$ and the frequency dependence of $Q$ is to place a series of receivers and a source on the same line. In this case a time source function called the Ricker wavelet is used. It is given by

$$R(t) = \{1 - 2[\pi f_s(t - 1/f_s)]^2\} \exp[\pi f_s(t - 1/f_s)^2].$$

(4.21)
Figure 4.10: Configuration used for the study of apparent attenuation. The star denotes the location of the explosion source, and the circles are the receivers. All edges have absorbing boundary conditions.

It can be considered to be equal to 0 outside the interval $[0, 2/f_s]$. This source is very interesting because its spectrum can be supported by the interval $[0, 3f_s]$, where $f_s$ is its predominant frequency.

The source is located at the center $O$ of the discretization grid which coincides with the origin of a Cartesian x-y coordinate system (Figure 4.10). The principle of this experimental procedure was based on the preconception that in cracked media, the intensity of the wave front should vary, on average, as

$$I(r, f) = \frac{I(0, f)}{r} \exp\left[\frac{-kr}{Q(f)}\right] \quad (4.22)$$

where $I(r, f)$ denotes the spectral density corresponding to frequency $f$ of the first-arrival part of seismograms recorded on receivers located at a distance $r$ from the source. Note that the factor $1/r$ is due to the geometrical spreading of the circular wave front in a 2-D medium. Here, $k = 2\pi f/v_p$ is the wave number associated
Figure 4.11: The least-squares regression for points \([r_i, \log[I_R(r_i, f)]]\) for the porous medium with porosity of 2.0%. Spectral density values, \(I_R(r)\), as a function of distance, \(r\), are shown for fourteen different values of frequency, \(f\).
with \( f \) and \( v_p \) is the velocity of the matrix. Now define \( D_A(r, t) \) as the average first-arrival signal over all the first-arrival signals recorded at receivers located a distance \( r \) from the source (see Figure 4.10). This could be justified because of the wavelength associated with \( f \), is much greater than the average radius of the cracks. The problem could be tackled from the angle of frequency dependence by Fourier-transforming signals \( D_A(r, t) \) into \( \tilde{D}_A(r, f) \). The spectral powers \( I_A(r, f) = |\tilde{D}_A(r, f)|^2 \) were then normalized by their counterparts \( I_H(r, f) \) defined in a homogeneous medium without cracks; this led to the ratios

\[
I_R(r, f) = \frac{I_A(r, f)}{I_H(r, f)}. \tag{4.23}
\]

The handling of these ratios was aimed at screening out the effect of geometrical spreading. Complicated as it might sound so far, this way of processing was in fact readily inspired by formula 4.22. Once the normalized average spectral power \( I_R(r, f) \) had been computed, its logarithmic version, \( \log[I_R(r, f)] \), was plotted versus distance \( r \) for each frequency. Through the cluster of points, a straight line could be drawn,
Figure 4.13: Four stacked seismograms for a medium with porosities of (a) 0.0%, (b) 0.5%, (c) 1.0% and (d) 2.0%, respectively. The waveform propagations through a porous medium are severely affected by the presence of the cracks. The wavelet becomes wider and lower in amplitude. Though the grain medium is totally elastic, the presence of cracks makes the medium behave viscoelastically because the cracks act as a low-pass filter.
Figure 4.14: Frequency evolution of the reciprocal quality factor, $Q^{-1}$, for a porous medium with porosity of 2.0%.

thanks to least-squares approximation. If the exponential form (4.22) holds, then the least-squares fitting must be "good enough", from then on, the slopes $\beta(f)$ of these lines were a rough measure of the attenuation rate per unit of travelled distance. In other words, the measured, frequency-dependent slopes $\beta(f) = -k/Q(f)$, enable us to deduce

$$Q^{-1}(f) = \frac{-\beta(f)}{k(f)} = -\frac{\beta(f)v_p}{2\pi f}.$$  

Examples of the least-squares regressions are shown in Figure 4.11 for a simulated porous medium with porosity of 2.0%.

4.3.3 Results

Four series of simulations were carried out on simulated rocks with fractal dimension $d = 2.5$, and various desired porosities. Figure 4.12 shows the example with porosity 2.0%, discretized on a 448 X 448 grid. The pore sizes are distributed between 3, 5 and 7 grids. The velocity of the grains was set to $v_p = 4000$ m/s. The discretization
parameters were chosen to $\Delta x = 0.2828$ mm and $\Delta t = 0.5 \times 10^{-5}$ ms so as to maintain accuracy for the numerical scheme. Figure 4.13 shows four stacked seismograms for the porous media with porosities of 0.0%, 0.5%, 1.0% and 2.0%, respectively. The waveform propagations through a porous medium are severely affected by the presence of the pores/cracks. Not only is the arrival time delayed but also the wavelet becomes wider and lower in amplitude and noise (Coda wave) present after the first break due to scattering from cracks. Though the grains of the media are total elastic, the presence of cracks makes the media behave viscoelastically because the cracks act as a low-pass filter, which is expected from Equation (4.15) of theoretical expectations discussed earlier. Moreover, the more the cracks, the more the viscoelastic effects. The velocity changes were measured using the picked traveltimes from data as in Figure 4.13, based on maximum absolute amplitudes and they are 1.4%, 2.2% and 3.6% for a medium with porosities of 0.5%, 1.0% and 2.0%, respectively. Their apparent attenuations were measured using the above described experimental procedure. The results obtained for porosity of 2.0% are displayed in Figure 4.14. As expected from the scattering-type mechanism discussed earlier, at sufficient high frequency (in comparison with the crack size), scattering effects are observed, and scattering induces an increase in attenuation with rising frequency at frequencies less than 60 kHz. After that the attenuation decreases with the frequencies. The maximum in attenuation occurs at wavelengths lower than the scatter size, the predicted value obtained from single scattering theory (Wu, 1982). One possible reason for this low prediction of the maximum is that multiple scattering needs to be considered.

4.3.4 Summary

We have successfully studied seismic wave propagation through cracked porous media using lattice Boltzmann acoustic model. The apparent attenuation obtained from simulations agrees with theoretical expectations.
Chapter 5

Summary, Conclusions and Recommendations

In chapter 2, we developed numerical schemes that use the lattice-Boltzmann technique to simulate single-phase flow, miscible displacement processes and immiscible displacement processes related to reservoirs. Technically, there are no difficulties to generalize these models to black oil models or composite models. However, practical implementation of these schemes for studies of small parts of reservoirs requires that they be extended to more complex problems through further research. On presently available hardware, we do not see them as directly applicable to full-field, three-dimensional studies that may have only a few cells between wells. In that context, they may be used indirectly to generate averaged properties for large cells that accurately reflect aggregate small-cell behavior, or high resolution simulations. The major advantage of the lattice Boltzmann method is its computational speed which is due to its intrinsic parallelism. Moreover, they are inherently simple and easy to implement. However, the price is its numerical inefficiency associated with very small time steps required by the stability limit. More work should be performed to make quantitative comparisons between lattice-Boltzmann simulators and those currently used in the reservoir industry. In particular, these comparisons should be carried out in terms of computational precision and efficiency.

In chapter 3, we described two lattice-Boltzmann computational models for seismic simulation. Numerical examples have demonstrated that the lattice-Boltzmann
method originally prescribed to solve Navier-Stokes equations can be an alternative numerical method to solve acoustic and elastic wave equations. Although the present lattice-Boltzmann method produces accurate results compared with analytical solutions, the lattice-Boltzmann kinetic equation is a numerical scheme of the first order in time and second order in space. In order to increase accuracy both in time and space, it would be desirable to develop a higher-order lattice-Boltzmann scheme. This is extremely important in 3-D simulations. The use of high-order methods permits the use of coarser grids and results in a potentially more efficient algorithm, since CPU time and I/O time may be more closely balanced.

Presently, no method is capable of modeling fluid flow and seismic waves through rocks with realistic microscopic features such as complex rock matrix, fractures and nonlinear-wave-induced fluid motions. However, it should be possible to develop a new simulation method with this capability based on modeling fluid flow and seismic waves using lattice-gas and lattice-Boltzmann methods. This approach may eventually lead to an improved understanding of how microscopic features in rocks relate to flow pattern, permeability, dispersion coefficients, seismic velocities and attenuation and, consequently, how to perform reservoir simulation and to interpret and invert seismic data. In chapter 4 we described such applications to calculate rock permeabilities and to study seismic attenuation. More work should be done along this direction. Hopefully such research will enable fluid flow and seismic waves to be simulated in a model obtained by digitizing a rock matrix given the properties of the grains and fluids in the pore space. Then, through studies of synthetics, one could numerically measure the transport and elastic properties of the rocks, providing a powerful analytical, as well as interpretive, tool for reservoir engineers and geophysicists.

Algorithm design needs to be re-evaluated with parallel processing in mind. The cellular-automaton methods presented in this thesis are one way to do this and could be the starting point for a new generation of methods for modeling of fluid flow and wave propagation in rocks.
Bibliography


