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APPLICATION OF THE LATTICE BOLTZMANN / LATTICE GAS TECHNIQUE TO MULTI-FLUID FLOW IN POROUS MEDIA

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The lattice Boltzmann approach to modeling fluid flow provides an efficient and reliable method for solving the Navier-Stokes equations and studying multi-fluid flow problems. In this paper, we report state of the art capabilities of our lattice Boltzmann simulator for single- and two-fluid flows in two- and three-dimensional problems. We review the development of the code and present some of the latest results. Some of the flexibility available in the model includes arbitrary pore space descriptions, wettability effects, surface tension relations, and chemical reactivity. Simulations of two-fluid flow through a digitized micromodel geometry, and through a high resolution, digitized sample of Berea sandstone are presented. Relative permeability as a function of wettability* and capillary number[†] is discussed. Integration of the lattice Boltzmann approach into larger scale models to build a more powerful tool for analyzing constitutive behavior is considered.

INTRODUCTION

Over the past twenty years the study of subsurface fluid flow has grown dramatically, in almost direct relation to the growth of computing power. Problems that were intractable twenty years ago are routinely solved today. We have reached a point where computing power is no longer a major restricting factor in tackling the majority of subsurface flow and transport problems. Yet, we remain perplexed as to how to model many systems - not computationally, but conceptually. Why is this? Our computing power has far surpassed our ability to gain understanding about the systems of interest. We can compute flow in a system that has a different permeability in every grid-block, but we are unable to physically determine what permeabilities to use at such a high resolution. We can write code to compute chemical reactivity, but we do not understand the physical processes that are occurring within the reactions, and so on. Data are being collected with ever increasing success, due to development of better technologies for sampling and

* Wettability is a measure of which of the fluids present in the pore space is preferably in contact the solid.

[†] Capillary number is a non-dimensional number that characterizes the relative strengths of viscous forces to interfacial tension forces in a given systems.

measurement, but it is neither feasible nor economic to continuously rely on physical measurement.

One means of potentially lessening our need for experimental data is to use a modeling approach that returns to first principles of physics. The growth of computing power has made it feasible to address questions regarding the influence of individual physical properties on fluid flow and transport behavior. Over the past eight years a computational approach that is particularly suited for studying micro-scale phenomena and relating them to continuum scale relationships has been under continuous development and extension. This approach is the "lattice gas" (LG) or "lattice Boltzmann" (LB) method.

What is a lattice gas / lattice Boltzmann? The LG method is a technique for simulating fluid flow which grew out of cellular automata theory. It is a temporally and spatially discrete method of reproducing fluid behavior. The LG method models a fluid as a collection of discrete particles moving through a space that is discretized by a regular lattice. These particles, which have unit mass and momentum, move through the lattice in a two-stage process. At each time step the particles advect to their next location ("streaming") then interact with other particles which occupy the lattice site ("collision"). Collisions are defined such that mass and momentum are conserved, and the averaged response recovers the partial differential equation of interest. For example, in the case of subsurface flow we are primarily interested in the Navier-Stokes equations. This approach is able to provide information on the microscopic scale, by looking at individual particle motion, and on the macroscopic scale, using ensemble averages of particle distribution and motion. Having the information at both scales simultaneously is important for improving our understanding of the constitutive parameters that are commonly used in large-scale simulations of flow and transport in porous media.

The LB approach is an extension of LG, in which the fluid is modeled using average particle populations, rather than discrete particles. The LB model still fully recovers the Navier-Stokes equations, however it eliminates the statistical noise inherent in the Boolean approach of the LG. Therefore, although the LB approach uses floating point operations instead of bit operations, the computational demands are balanced by the elimination of Monte Carlo-type runs to obtain a smooth, average solution.

Frisch, Hasslacher, and Pomeau, in 1986, introduced the first LG model that recovered the correct hydrodynamics. The "FHP" model is a two-dimensional, single-fluid flow model using a triangular lattice and up to six particles per lattice site (corresponding to up to one particle per link). This model was extended to three dimensions in d'Humieres et al. (1986) and Frisch, et al. (1987), using a face-centered hypercubic (FCHC) lattice with up to twenty-four particles per lattice site. The FHP model continues to be the foundation for LG codes.

Chen et al. (1992) introduced a LB model with two particles speeds that was able to utilize a true 3-D lattice which made it possible to have only fourteen nearest neighbors, as opposed to twenty-four. This significantly reduces the required computation time.

Rothman and Keller (1988) extended the single-fluid FHP model to simulate multi-fluid flows by introducing particles of two "colors". Each particle continues to follow the same collision rules as in the single fluid model except at interfaces. At interfaces the collision rules change to redistribute colors such that particles of the same color tend to remain together. Chen et al. (1991) and Somers and Rem (1991) modified the two-fluid approach, using both colored particles and colored "holes", where a "hole" denotes where a particle previously resided. This modification results in a more computationally efficient collision process at fluid-fluid interfaces.

Lattice gas automata have proven to be especially successful for describing flows through porous media because of the ease with which complex geometries and corresponding boundary conditions are handled. LG/LB methods have also been successfully applied to other subjects, including chemical reactivity (Wells et al., 1991; Gabetta and Monaco, 1991; Dawson et al., 1993), magnetohydrodynamics (Chen et al., 1991), miscible displacement (Holme and Rothman, 1992), non-Newtonian fluids (Aharanov and Rothman, 1993), and thermohydrodynamics (Alexander et al., 1993).

THE LATTICE BOLTZMANN FLOW SIMULATOR AT LOS ALAMOS NATIONAL LABORATORY (LANL)

We believe that the LANL simulator the most complete and efficient LB model currently in existence. LANL is also fortunate enough to have massive computing power in its 1024-node massively parallel Connection Machine 5 (CM-5, by Thinking Machines) not equaled anywhere else. The LG and LB schemes are intrinsically parallel, making implementation on a massively parallel computer easy and efficient. The efficiency of implementation and storage allows very high resolution of many complex systems. This combination of code capability and computing power provides a formidable tool for studying the fundamental processes involved in multi-fluid flow and transport.

The LANL model is based on the FHP work in 2-D. The model uses the expanded 3-D capabilities of the 2-speed, 14-neighbor lattice of Chen et al. (1992). Multiple fluids are implemented based on Gunstensen et al. (1991) with modifications described by Grunau et al. (1993) to more efficiently model fluid interfaces. Further extensions have been made and reported (Grunau, 1993) that allow arbitrary viscosity and density ratios for the fluids, and arbitrary interfacial tensions.

The model is capable of simulating flow of one to three (or more) fluids in two or three spatial dimensions. Domain sizes as large as 256^3 lattice sites have been run. The 256^3 lattice corresponds to an actual high resolution digitization of a 2 cm^3 sample of Berea sandstone obtained through micro-computed tomography.

The LB model allows for arbitrary porous medium characteristics. This includes an arbitrarily complex pore geometry, including surface roughness. It is further possible, with the current code, to define arbitrary surface wettability and/or mineralogy, discretized as finely as one lattice site. Tests of the code have shown it can reproduce contact angles ranging from 20° to 180° . This range is sufficient to allow simulation in

the entire range of fluid-pair wettabilities. Specification of mineralogy is of interest when modeling chemical reaction processes.

Options for boundary conditions for the inlet and outlet faces include: fixed pressure drop, fixed inlet and outlet density, and fixed input velocity (Dirichlet condition). Top and bottom boundaries are assigned to be either periodic or no-flow.

The LANL LB model is also able to implement almost arbitrary fluid characteristics. As all values in the LB methods are dimensionless, fluid characteristics are all defined in terms of ratios. Viscosity ratio, density ratio, and interfacial tension are all specifiable by the user. The only limitation on the choice of these values is in how that choice affects simulation run time. An increase in density ratio of one order of magnitude corresponds to approximately doubling the necessary run time.

The LB simulator provides a variety of output information. Both local and averaged velocities, pressures, and momenta are given. Fluid distributions and bulk saturations are provided, and relative permeabilities are computed. All averaged information is calculated as a straight summation over the probability distributions for each link of each lattice site. Relative permeabilities are computed based on the formulation given in de Marsily (1986).

Another area of effort that we have been focusing on with the LB/LG models is of coupled flow and chemical reactions. We continue to develop our LG and LB hydrodynamic models which integrate chemical transport and reaction processes for application to study at the pore scale. These models are partially distinct from the general multi-fluid models. The chemical reaction models incorporate most of the flexibility of the multi-fluid models but are currently simplified to two dimensions to allow for the increased computationally requirements. Diffusion, sorption and desorption, and solutions and dissolution are incorporated into the models. Sorption and desorption reactions are the focus of work with fixed boundary conditions between solution and solid (Wells et al., 1991; Janecky et al., 1992). Initial detailed models have been developed for sorption/desorption chemical reactions at solid surfaces (Janecky et al., 1993), including multicomponent sorption/site competition as a function of space and time in heterogeneous pore network structures, where hydrodynamic transport, solute diffusion and mineral surface processes are all treated explicitly. The present LB-chemistry model includes potential for up to 200 solute components and binary solute reactions (Dawson et al., 1993).

RESULTS FROM THE LANL LATTICE BOLTZMANN SIMULATOR

Our recent work has been primarily directed toward the application of the LB method to simulation of constitutive relationships in porous media. We began by simulating single fluid flow through a variety of porous media and computing permeabilities for the media. Both 2-D (micromodels) and 3-D (beadpacks, actual porous samples) systems were simulated. Simulations were run in digitizations of actual porous media, which made it possible to closely compare simulated and measured permeabilities. Table 1 contains values for measured and calculated permeabilities in a number of different porous media.

The agreement between simulated and measured permeabilities is excellent. There is one notable difference for the sandstone simulated in the short direction of the core. The discrepancy between the two values is most likely due to the subsample from which the digitization was made not being homogeneous at the scale of the simulation, while the larger experimental sample was homogeneous. This raises the question of how large a simulated domain must be, and to what resolution must we discretize to obtain a representative pore space. Current considerations of these questions is considered in the last section of this paper.

Porous Medium	k (exper.) [darcy]	k (simul.) [darcy]	Imaging Resolution	Comments
Micromodel-1	23	21.5	~80 μm	pore depth=50 μm
Micromodel-2	37	32	~80 μm	pore depth=74 μm
Beadpack	1100	1000	50 μm	
Berea	1	1.2	10 μm	
Sandstone	7.4	8.6	20 μm	flow in long dir
Sandstone	7.4	21.5	20 μm	flow in short dir

Table 1: Comparison of measured and calculated permeabilities for various porous media

Simulations have also been run for two-fluid flow, from which the corresponding relative permeabilities have been computed. Both 2-D and 3-D systems have been used, but figures are selected from 2-D systems for ease of graphical presentation. Examples of some of the model results are shown in Figures 1 and 2.

We are not only interested in being able to reproduce the appropriate functional response, but also in identifying what influence various physical features and flow processes have on the constitutive behavior. With the two-fluid systems we have also addressed the question of how wettability and capillary number (N_{ca}) affect displacement efficiency and permeability. Figure 1 shows fluid distributions in a digital micromodel pore space for flows at three capillary numbers. In Figure 1a the flow is in a viscous dominated regime, reflected by more frontal displacement and high displacement efficiency than the other figures. In Figure 1c the flow is in an interfacial tension dominated regime, which is reflected in the highly fingered fluid distribution, and the high residual saturations. Figure 2 shows the corresponding calculated relative permeability curves for the systems run at the larger two of capillary numbers.

The LB simulator is capable of capturing a range of rock wettability between 20° and 180° . This range is sufficient to be able to capture the entire range of wettability, in conjunction with the model ability to change the surface wettability. Figure 3 plots the displacement efficiency versus the wettability. The most efficient displacement is obtained at neutral wettability, and it is most difficult to extract oil from oil-wet rock.

Figure 1. Comparison of immiscible displacement under different capillary number (velocity) drives. White is non-wetting. Gray is wetting. a) $N_{ca} = 2.2 \times 10^{-2}$; b) $N_{ca} = 5.7 \times 10^{-3}$; c) $N_{ca} = 1.5 \times 10^{-4}$

Figure 2. Relative permeabilities for micromodel simulations.
a) $N_{ca} = 10^{-2}$, b) $N_{ca} = 10^{-3}$

Figure 3. Effect of wettability on residual oil saturation from a simulated waterflood in a micromodel (water displacing oil).

MOVING BETWEEN MODELING SCALES

We are beginning to address the question of moving between scales of fluid flow using LB techniques. Although the LB method uses averaging to provide any macroscale information, i.e. pressure and velocity fields, the resulting averaged quantities must be representative of the simulation domain to be of value. It is not clear, at this time, whether these averaged quantities values can be extrapolated beyond the simulation domain. We must first determine appropriate averaging volumes and geometries for use in paralleling classical averaging theories. It should be kept in mind that the particular REV size may vary between different extensive variables.

We are currently trying to quantitatively describe the influences of different system properties to arrive at descriptive parameters that can be used to synthesize new, physically based functional forms for constitutive relationships. We are examining how pore structure, material texture, and fluid-solid interactions affect the definition of characteristic medium constants or responses (such as the porosity, permeability, relative permeability, wettability, dispersivity, etc.). This will help to identify a true REV. We anticipate paralleling common theoretical procedures by integrating, pore-scale quantities obtained from simulations (such as specific volume, specific interfacial area, fluid mass density, fluid momentum density, etc.) over predetermined REV's, thus computing typical macroscopic quantities (saturation, flux, interfacial area per unit volume) that are usually measured experimentally, and applied in field scale equations.

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