LA-UR-96- 3 4 5 6

Title: Developing the R&D 100 Award-Winning Lattice Boltzmann Permeameter Toward a Marketable Product

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OCT 30 1996

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Submitted to: DOE Office of Scientific and Technical Information (OSTI)

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Form No. 836 R5
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Developing the R&D 100 Award-Winning Lattice Boltzmann Permeameter Toward a Marketable Product

Wendy E. Soll*, Shi-Yi Chen, Gary D. Doolen, and Kenneth G. Eggert

Abstract

This is the final report of a one-year, Laboratory-Directed Research and Development (LDRD) project at the Los Alamos National Laboratory (LANL). Computational models of oil, gas, and water flow through porous reservoir rock are used in reservoir management to decide whether or not, and how, to develop and produce hydrocarbon reserves. The flow models have major impact on these decisions so their accuracy, cost, and speed is paramount. The accuracy of the flow models is strongly dependent on the accuracy of the physical characterization of the reservoir rock's pore-fluid system. System characterization is typically done in the laboratory. As an alternative, we have developed a numerical approach for determining the constitutive information. The project sought to use computational techniques that could incorporate all of the basic physical processes that influence fluid movement through the porous rock yet remain computationally efficient. The lattice Boltzmann (LB) numerical technique fits these requirements, and is able to incorporate complex pore geometries exactly and reproduce behavior of multiple fluids. The flexibility of the LB approach allows the numerical model, called the lattice Boltzmann Permeameter (LBP), to determine constitutive relationships (i.e., relative permeabilities) over a much wider range of conditions than can be achieved in a laboratory. Our project was directed toward improving the LBP to make it available to a wide range of users. Improvements were made in computational speed and efficiency, user interfaces, and visualization capabilities.

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1. Background and Research Objectives

Computational models of oil, water, and gas flow through porous reservoir rock are used in reservoir management to decide whether or not, and how, to develop and produce hydrocarbon reserves. Ground water remediation and site assessment are described by the same set of equations as oil and gas production and are subject to the same challenges in understanding the system. The accuracy of field-scale flow models is strongly dependent on the accuracy of the physical characterization of the reservoir rock's pore-fluid system. Characterization includes properly representing the porous medium, the fluids, and the interactions between the medium and the fluids, all of which is a very difficult task. Historically, reservoir (aquifer) characterization has been obtained through laboratory and field measurements. Such experiments are not only time consuming and expensive, but also capture behavior at a scale that has already averaged out the significant properties that govern fluid behavior. As a result of measuring averaged properties, it has not been possible, up to this point, to predict system characteristics accurately based on knowledge of the geology and the fluids present. Efforts to accurately model or predict fluid movement in porous media thus continue to be bound by the need for such measurements.

There are many industrial and environmental situations that are concerned with fluid movement through porous media. Examples of such situations include: enhanced oil and gas recovery, ground water contaminant remediation, gas and water flow in concrete, composite materials forming, and biomedical applications (i.e., osmotic materials and transport through human tissue). The role of microscale modeling and analysis in understanding flow in these complex systems has grown tremendously over the past few years. Much of this growth has been driven by two factors: the lack of success in improving understanding through more traditional scientific/modeling methods and improvements in computational and experimental capabilities making microscale modeling feasible. Los Alamos researchers have been integral to the development of pore-scale modeling of flow in porous media through lattice-gas and lattice-Boltzmann methods (i.e., Frisch, *et al.*, 1987; Chen, *et al.*, 1989; Chen, *et al.*, 1991; Grunau, *et al.*, 1993; Dawson, *et al.*, 1993). Furthermore, the computing power initially available through LANL's CM-2 computer and now the CM-5 computer has been instrumental in extending these modeling techniques to application to physical problems.

The primary objective of our effort is to improve simulation capability for multiphase porous media flow by developing numerical techniques to determine system characteristic properties directly from the fundamental physical processes that govern the system. We focus on the pore scale, where we can apply the non-averaged continuum equations. By returning to the fundamental micro-scale processes we can incorporate all of the physics that influence the

fluid behavior and, as a result, develop an extremely accurate and versatile model. The information at the micro-scale is then "averaged" to obtain information at a larger, continuum scale, as required by reservoir models.

The overall goal of this project was to improve the capabilities and efficiency of the LANL lattice-Boltzmann (LB) multiphase-flow code, the 1994 R&D 100 Award-winning lattice-Boltzmann Permeameter (LBP), to an extent that it is an effective numerical tool for determining constitutive relationships and system parameters for input to reservoir-scale numerical codes. The goal was approached through (1) improving the accuracy and efficiency of the LB code itself, (2) developing an upscaling approach that incorporates the pore-scale data generated by the LBP into information at a slightly larger scale (i.e., laboratory core) that is useful to existing field scale simulators, and (3) using simulation results to analyze flow response as a function of specific system conditions. This work has the potential to impact our understanding of fundamental physical processes in porous media flow and expand our ability to capture characteristic behavior of a porous medium-fluid system. One example is the lattice-Boltzmann Permeameter's (LBP) application to enhanced oil and gas recovery. Our numerical model is the first tool that makes it viable to determine permeability of porous media to fluids at the high spatial resolutions desirable for basin-scale modeling. Our LBP is also the only tool that makes it possible to determine relative permeabilities under a variety of system conditions. The LBP also provides a means to understand how different aspects of the porous medium system affect the relative permeability relationship. With our model it is possible to identify characteristics of the system that prevent flow or that enhance flow, such as mineralogy changes. Such insight can be critical to obtaining good oil production or contaminant remediation, where one is dealing with real systems that may change faster spatially and/or temporally than is possible to capture in the laboratory.

2. Importance to LANL's Science and Technology Base and National R&D Needs

This project has applications to many R&D areas of national interest and ties in to many key areas of LANL's science and technology base. It combines some of the leading thinking in advanced theoretical physics, utilization, and extension of massively parallel computing capabilities and visualization techniques and application of these capabilities to solving real-world problems. It also provides an excellent approach to advancing scientific understanding of multiphase flow and transport processes in complex flow domains. This project supports Los Alamos core competencies in theory, modeling, and high-performance computing as well as earth and environmental systems.

3. Scientific Approach and Results to Date

The lattice Boltzmann Permeameter uses the lattice Boltzmann numerical approach for modeling hydrodynamics at the pore-scale to identify important characteristics of the porous medium, the fluids, and the interactions between the two. The recent development of the LB method has provided new computational schemes for solving a variety of partial differential equations (PDEs) and modeling flow through porous media. Lattice methods are a powerful alternative to traditional numerical schemes for solving PDEs and modeling physical systems. In finite-difference and finite-element methods the given macroscopic equation is solved by some specific numerical discretization, while in full molecular-dynamics descriptions each individual particle is closely and accurately followed. Unlike these traditional numerical schemes, the idea behind the lattice method is to construct a simplified particle-based process so that the macroscopic averaged properties obey the desired macroscopic equations. The utilization of the particle description of the kinetic equation provides some of the advantages of molecular dynamics, including clear physical pictures, easy implementation of boundaries, and fully parallel algorithms, while retaining computational tractability. 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.

A common feature of the LB method is the discretization of space and time. Lattice methods are purely local, parallel, and very fast. In the LB method, space and time are discrete. Real numbers represent the local ensemble-averaged particle distribution functions and only kinetic equations for the distribution functions are solved. An important property of lattice methods is that while all other methods are unable to model complicated geometries efficiently, the LB model naturally incorporates arbitrarily complex domain geometries. This makes lattice methods more suitable for simulating flows in systems such as porous media. Because of its ability to represent the exact Navier-Stokes equation in a parallel fashion, to handle arbitrary complicated geometry, and simulate surface dynamics and wettability, the LB method is becoming an increasingly popular means of modeling multiphase fluid flows in porous media.

This work focused on improving and enhancing the LBP multiphase flow in porous media code. This model is capable of simulating three-dimensional flow of up to three fluids. The LB model allows for arbitrary porous medium and fluid characteristics. Adjustable characteristics include arbitrarily complex pore space geometries, arbitrary densities,

viscosities, interfacial tensions between fluids, contact angles, and boundary conditions. Currently, output options include both local and averaged velocities, pressures, and momenta. Fluid distributions and bulk saturations are provided and relative permeabilities are computed. (Further description of the work can be found on our home pages, see references for world-wide web addresses). In principle, these capabilities provide the flexibility to examine a wide range of processes encountered in enhanced oil recovery and environmental problems involving non-aqueous phase liquids in ground water.

Many improvements have been made to the LBP code to make it more generally useful. Requiring a massively parallel computing platform was a limiting factor in accessibility to the user. Over the past year we have developed a distributed-computing version of the code, which is able to run on workstation networks as well as parallel computers that operate as distributed environments (IBM SP2, Cray T3D, TMC CM-5). Benchmarking of the distributed computing version showed that a 16-node IBM SP-2 has comparable or better speed than a 256 node TMC CM-5. Run time on a network of workstations will be somewhat slower than for the massively parallel systems and domain size will also be reduced due to limits in memory (each CM-5 node has 32 MB of memory). However, we anticipate that in many cases, particularly given implementation of upscaling methods, it will not be necessary to run large systems, and so the benefit will be derived from having access to this numerical tool.

A second objective was to increase code efficiency. This allows larger system sizes to be run, better discretization of the pore space, and less computer use. A number of improvements to the LB tool for speed and accuracy have been implemented. We have tested a new method for handling boundaries (walls) that is second-order, space-and-time accurate, replacing a first-order-accurate method. The second-order-accurate boundary condition also greatly extends the range of viscosity ratio (fluid a/ fluid b) that can be efficiently simulated. A new approach has been designed for recovering interfacial tension at fluidfluid interfaces, which is a factor of five faster than the previous approach. We have compared three different methods for handling fluid-fluid interfaces to determine each method's ability to capture critical interface behavior and to identify the different ranges of interfacial tension obtainable.

A third objective was to implement upscaling methodology to move from the pore scale to the core scale. We have worked on two approaches to upscaling. One method is based on a new approach to the multiphase flow equations and requires additional information on interfacial area between fluids and solids. We have implemented all of the necessary code for this method. The other approach applies renormalization group theory, which calls for grouping small subsets of known quantities. One difficulty is in being able to define appropriate averaging volumes and geometries. A key concern is whether enough pore data is available to define sufficiently large representative volumes or whether a need exists to model

or extrapolate pore geometries with fractal or other statistical techniques. Simulations using pore spaces from high resolution micro-computed tomographic images of producing reservoir rocks indicate that even very small samples (1 cm^3) may have two or three regions of different effective permeabilities.

In conjunction with code development, we have been applying the LBP toward our last objective: to examine how pore structure, surface properties, and fluid-solid interactions affect the definition of characteristic system response (such as permeability, relative permeability, dispersivity, etc.). The role of wettability of the rock surface is important because it is not well known, can vary temporally as well as spatially, and is generally assumed to be strongly water-wet (prefers contact with water over other fluids). Simulations run to test the effect of wettability have indicated that while relative permeabilities of oil appear to be sensitive to wettability for partially oil-wet media, relative permeabilities of water do not appear overly sensitive. This result may provide some insight into the role of fluid transport through thin films.

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