Understanding and predicting physical properties of rocks through pore-scale numerical simulations

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공극스케일에서의 시뮬레이션을 통한 암석물성의 이해와 예측

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Abstract : Earth sciences is undergoing a gradual but massive shift from description of the earth and earth systems, toward process modeling, simulation, and process visualization. This shift is very challenging because the underlying physical and chemical processes are often nonlinear and coupled. In addition, we are especially challenged when the processes take place in strongly heterogeneous systems. An example is two-phase fluid flow in rocks, which is a nonlinear, coupled and time-dependent problem and occurs in complex porous media. To understand and simulate these complex processes, the knowledge of underlying pore-scale processes is essential. This paper presents a new attempt to use pore-scale simulations for understanding physical properties of rocks. A rigorous pore-scale simulator requires three important traits: reliability, efficiency, and ability to handle complex microstructures. We use the Lattice-Boltzmann (LB) method for single- and two-phase flow properties, finite-element methods (FEM) for elastic and electrical properties of rocks. These rigorous pore-scale simulators can significantly complement the physical laboratory, with several distinct advantages: (1) rigorous prediction of the physical properties, (2) interrelations among the different rock properties in a given pore geometry, and (3) simulation of dynamic problems, which describe coupled, nonlinear, transient and complex behavior of Earth systems.
Keywords : pore-scale simulation, physical properties, lattice-Boltzmann, FEM, nonlinear, transient, complex behavior of Earth system

요약 : 지구과학은 지구와 지구시스템을 기술(description)하던 기존의 역할에서 벗어나, 진화하는 지구 시스템 안에서 일어나는 프로세스의 모델링(process modeling), 시뮬레이션

(simulation) 그리고 이러한 현상들을 구상화(visualization)하는 방향으로 그 접근 방법이 서서히 그러나 매우 역동적으로 변화하고 있다. 하지만 이러한 모델링 및 시뮬레이션은 현대의 컴퓨터 기술의 발달에도 불구하고 그 수행이 쉽지는 않다. 그 이유로는 지구의 현상들은 그 현상의 기초원인이 되는 물리적 · 화학적 프로세스들이 비선형적이며, 서로 다른 프로세스들이 상호 연동되어 발생하고, 시간에 따라 변화를 보이기 때문이다. 더구나 이러한 복잡한 프로세스들이 암석의 공극구조라는 매우 복잡한 구조 안에 일어날 때, 그 현상의 모델링 및 시뮬레이션은 그 어려움이 더욱 커지게 된다.따라서 이러한 지구시스템의 여러 가지 프로세스들에 대한 효과적인 모델링 및 시뮬레이션을 위해선 지구의 기본 구성단위인 암석의 구조, 즉 복잡한 공극구조의 이해 및 그 형태를 효과적으로 컴퓨터상에서 수치적으로 기술하는 방법의 개발이 선행되어야 한다. 본 발표에서는 이러한 공극스케일의 모델링을 위한 격자볼츠만 방법, 유한요소법을 이용한 수치방법과 그 결과와, 지구의 여러가지 비선형적이고 시간종속적인 프로세서의 모델링에의 응용가능성에 대한 내용을 제시한다.
주요어 : 공극스케일, 수치모델링, 암석의 물성, 격자볼츠만 방법, 유한요소법, 비선형, 시간종속적인 지구의 프로세스

1. Introduction

This paper presents pore-scale simulation techniques on predicting physical properties of rocks using Lattice-Boltzmann method for fluid flow in porous media and finite-element method for electrical and elastic properties of rocks. Numerical experiments were performed in a digital rock sample from X-ray micro-tomography. Brief details of numerical methodology and results of physical properties of rocks, such as permeability, relative permeability, electrical conductivity and elastic moduli will be presented. The strength of our approaches are (1) robust prediction of physical properties, especially for those that are very difficult to measure in lab, and (2) interrelation between different properties because our numerical simulators do not need modification or simplification of pore geometry of rocks. Finally, we will briefly mention the applicability of our numerical framework (computational rock physics; Fig. 1) to nonlinear, complex and transient processes of evolving Earth, such as changes in physical properties of rocks during diagenesis, formation of gas hydrates or multiphysical phenomena, e.g. transport properties in partially-saturated rocks.

2. Lattice-Boltzmann Flow Simulation

The Lattice-Boltzmann (LB) method is based on cellular automata theory, which describes a complex system by the interaction of a massive number of particles following simple local rules (Doolen, 1990; Chen et al., 1992; Chopard and Droz, 1998). Although the particles have nearly nothing in common with real fluids, the rules in the Lattice-Boltzmann method recover the Navier-Stokes equations at the macroscopic scale (Ladd, 1994; Rothman and Zaleski, 1997). While other methods, such as network models, the FEM or the FDM, discretize the model and the

governing equations, the LB method recovers the governing equation (Navier-Stokes equations) from rules in the discrete model. This gives the biggest advantage of the Lattice-Boltzmann method that it is readily applied to any arbitrary discrete geometry (Ladd, 1994; Martys and Chen, 1996; Keehm et al., 2001). In addition, it describes fluid flow in porous media very accurately. This strength comes from the characteristics of the LB algorithm. (Keehm, 2003) Another advantage of the LB method is that the implementation is very simple, and portable for different computer platforms. It is also ideal for parallel implementation, since most operations in the LB method are local. For certain applications, such as multiphase flow in porous media, there is a growing consensus that the LB method is a strong contender for the best fluid-simulation approach currently available (Fredrich et al., 1999; Succi, 2001). Details on algorithm and implementation can be found in Ladd (1994) and Keehm (2003). Fig.2 shows an example of fluid flow in porous media and predicted permeability from the simulation. Fig. 3 shows two-phase flow in pore geometry and relative permeability of Fontainebleau sandstone.

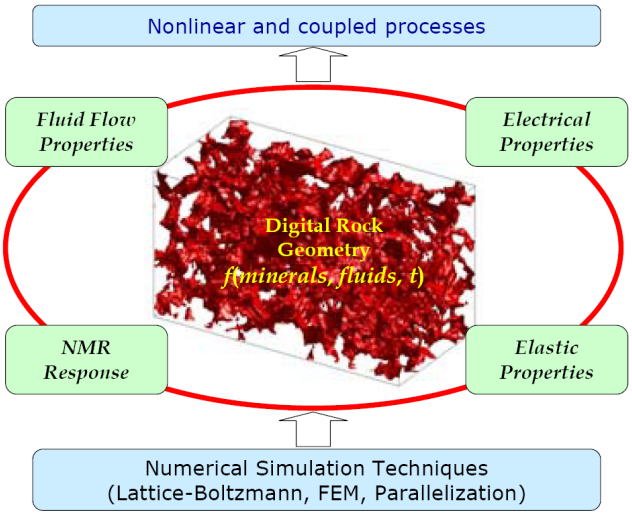

Fig. 1. Schematic diagram of the computational rock physics framework.

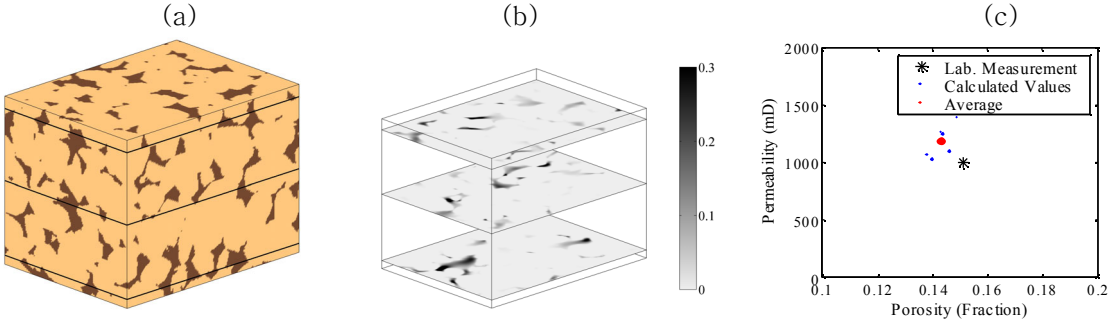

Fig. 2. (a) A 3D pore structure from digital Fontainebleau sandstone with 15% porosity. (b) Local fluid flux from flow simulation at selected cross-sections. (c) Permeabilities from laboratory measurement (star), from the LB flow simulations (red dot).

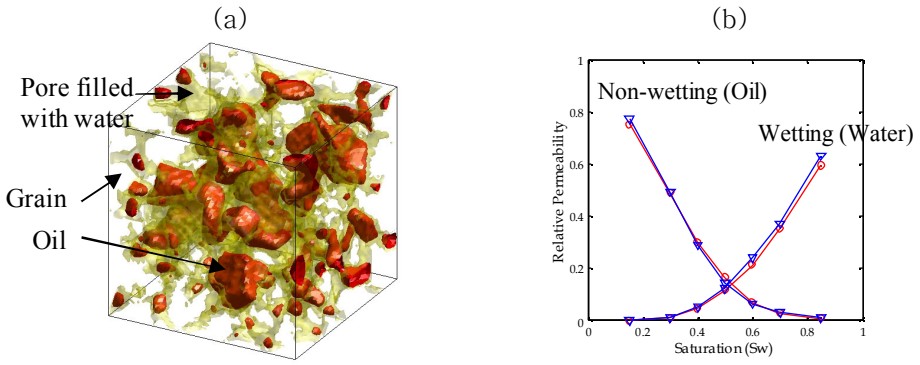

Fig. 3. (a) Two fluids after two-phase flow simulation. (b) Relative permeability curves from two different subsets of the digital Fontainebleau sandstone samples.

3. Finite Element Method for Electrical and Elastic Properties

The theory on the finite element programs basically follows Roberts and Garboczi (2002). The essential idea is that a variational principle exists for the linear elastic problems. For a given microstructure, subject to applied fields or other boundary conditions, the elastic displacement distribution is such that the total energy stored in the elastic case, is extremized, such that the gradient of the energy with respect to the variables of the problem (elastic displacement) is zero. Since we want to use FEM model for many different rocks (structures), we tried to avoid extensive meshing procedure. Hence we use the trilinear grid structure on our FEM modeling. Fig. 4 shows local electrical current from FEM simulation and its comparison with fluid flow result. We clearly see the fluid flow is affected much more by the grain-pore boundary than electrical current. Fig. 5 shows results from elastic simulations, which were obtained from uniaxial strain tests. We changed porosity or the sample by enlarging the grains. The figure also shows the elastic property of each sample, i.e. seismic velocity. The results were compared against the laboratory data and both agree each other very well.

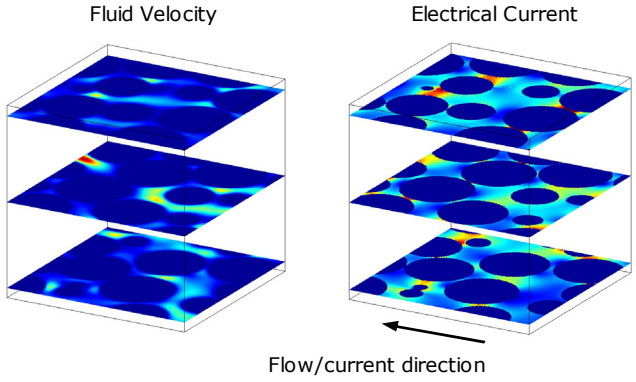

Fig. 4. Fluid velocity from flow simulation (left) and electrical current from FEM electrical conductivity simulation (right). Red denotes high values and blue shows low values.

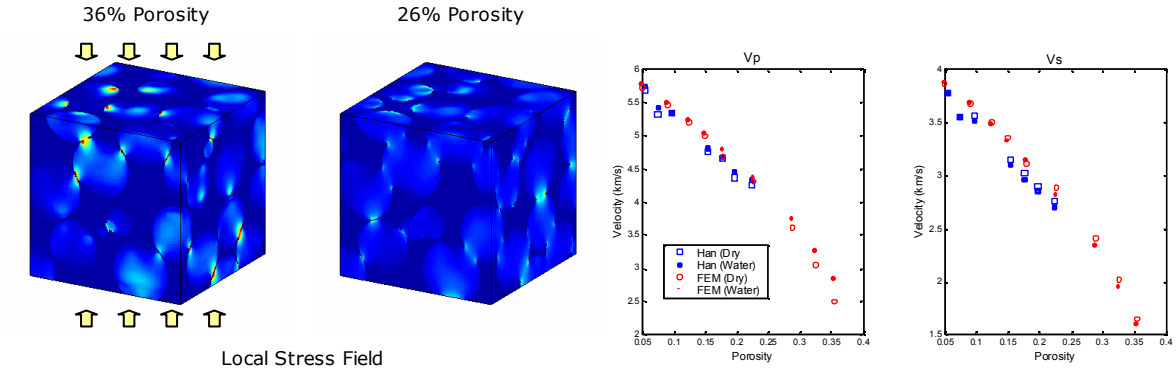

Fig. 5. Uniaxial strain tests for rocks with different porosity. Left figures show the local stress concentration and right figures show calculated velocities(red) and lab measurements(blue).

4. Applications of Pore-scale Simulators

These robust pore-scale simulators can be applied to many different areas. We have shown that these simulators are very useful for diagenesis modeling (Keehm et al., 2001). Our framework could give the evolution of physical properties, such as permeability and resistivity during diagenesis. In this paper we show one example - transport properties in partially-saturated rocks. Fig. 6 shows what happened in rocks with partial saturation. With very small amount of water, water phase will be isolated at the pore throat. With increasing amount of water, the water phase connects through the sample (water percolation) at some point. If the water(brine) phase is conductive, we will observe a jump in electrical conductivity. With more water, at a certain point, the air phase can lose connectivity, thus air permeability will steeply decrease (air percolation). This phenomenon involves many different physics: two-phase flow simulation; electrical conductivity simulation; and air permeability simulation. Our simulations successfully calculated transport properties in this multiphysical process.

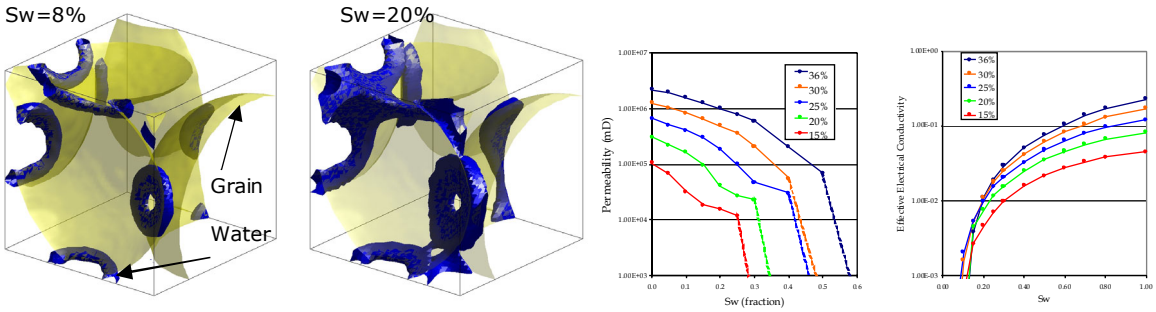

Fig. 6. Partially-saturated rocks (left) and permeability and electrical conductivity changes by saturation changes.

5. Conclusions

We presented the basic idea about pore scale simulation framework, so-called computational rock physics. Currently, single-phase and two-phase Navier-Stokes solver using the LB method, electrical and elastic property simulators using FEM, and NMR response simulation using random-work and the LB are available. These simulators are ready for complex pore geometry and we can predict interrelations of physical properties of rock since they use common digital pore geometry without modifications or simplifications of pore structures. We have shown one application example of this framework and its applicability. With the pore-scale simulation framework, we can perform many multiphysical process modeling including gas hydrates formations and physical property changes.

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