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Numerical modeling of the carbonate and the sandstone formations

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Abstract

It is of interest in various scientific and industrial contexts to make a reliable estimation of the transport properties of porous media via more accessible probes such as NMR that yield information on static pore geometry and porosity. When the pore geometry is simple, there are empirical recipes that have long proven reliable in bridging the gap. For heterogeneous systems, such recipes fail to give a consistent prediction and invite case-by-case modifications. This is just one of many indications that the complex pore geometry erodes the predictive power of empirical laws that work well in simpler situations. Heterogeneity combined with sizeable diffusive coupling in extended pore space further undermines the validity of the MR interpretation based on simple pore geometry. On top of this, possible spatial variation of surface relaxivity may further complicate the interpretation. Resolution of these issues for real life samples requires elaborate simulations in tandem with experimental verifications on the shared pore geometry. We report on a recent progress which allows combined parallel Lattice Boltzmann and random walk simulations to study transport and diffusion properties in various types of pore geometry, from simple 2D micro-fluidic mazes, 3D glass-bead packs and sandstones to more complex carbonates.

Keywords

Diffusion Lattice-Boltzmann NMR Rock Flow-propagator

1. Introduction

As the fidelity of numerical modeling techniques reaches the level where quantitative comparison with experimental data is feasible, they are used in *virtual* experiments [1] to reveal what is going on under the resolution-imposed veil for a given probe inside a porous medium. To be specific, we aim to improve on the cross-correlation between the transport and the diffusive properties of fluid in complex porous media. The *complex* refers specifically to the presence of multiple length scales in the pore geometry within accessible distance for a given probe. Ultimately, we aim further for the *complex* (i.e. multi-phase and multi-component and non-Newtonian) fluid dynamics in such a *complex* static environment. But it is worthwhile to pause and retool various theoretical notions that, while having been extremely effective for simple and periodic porous media, leave a significant gap facing the

complex pore geometry and fluid configurations. These include the direct mapping between MR relaxation spectrum and the pore size distribution, the assumption of uniform surface relaxavity, or the physical nature of distinct flow patterns in complex pore/fluid configurations, just to name a few. The aim of this report is not to provide answers to these issues, but to present a working numerical approach specifically developed with a view to help slay the beast one head at a time in a manner and scale that have not been easily available in the past.

2. Numerical Methods

We describe, in four steps, a numerical simulation program based on modern programming techniques [2] for parallelized modeling of diffusion and flow in general porous media.

2.1. Pore generation and structure analyses

The digital pore space may be constructed out of various sources such as tomograms [1], standard image files and geographical maps, and also via prescribed algorithms that control the hierarchical distribution of porosity at different length scales. This latter capability provides a *minimal* model to capture essential complexity in the carbonate rocks. Two-point pore/grain correlation functions, local magnetic field, cluster identification, erosion length [3], and fractal analysis are among the built-in methods applied to the digital pore structure. For high-resolution tomograms, some of these algorithms were modified to take advantage of parallelism and hierarchical pore structure, and to break the 32-bit addressing limitations.

2.2. Parallel Random walks for NMR and diffusion modeling

At the simplest level, random walks with a continuous step size distribution in three orthogonal directions are performed with stochastic killing at interfaces as a way to simulate the basic magnetic resonance response of the pore filling fluid. The killing probability (related directly to surface relaxivity ρ) may be designed to vary with position. [3] The algorithm is parallelized via allowing the migration of walker objects across the network. Consistent and efficient synchronization is achieved via a combination of multiple threads and notification mechanisms and parcelled transmission of consolidated migrant walkers. Up to 10^6-10^7 random walkers can be employed simultaneously on networked desktop systems and their evolution interactively controlled and visualized. The diffusion constant may also vary among different species of walkers or depending on the site (in the case of static water-oil configurations) with adjustable transmission properties through the interfaces. We apply these techniques for direct MR response modeling in parallel with experiments done on the specimen from which the digital pore space is generated. We probe the effect of spatially varying ρ on the time domain magnetic relaxation [3], their coupling with the pure pore geometry-, and diffusive coupling- effects, time-dependent diffusion coefficient $D(t)$ and its cross-correlation with other properties such as the T_2 relaxation time of walkers and distance to the nearest wall at t =0.

2.3. Parallel Lattice Boltzmann simulations

The standard 3D lattice Boltzmann (LB) algorithm is parallelized and implemented for the simulation of a single component flow; modules for an multi-component LB is under development. Efficient inter-processor coordination is handled via control objects that reside in each machine and carry out packing and mapping of boundary ("*ghost"*) cell data via various distributed objects [2] communication methods. From the LB simulations, we obtain the permeability and the local flow velocity profiles in porous media on which we also perform diffusion-MR simulations for cross-correlation between the transport and MR responses.

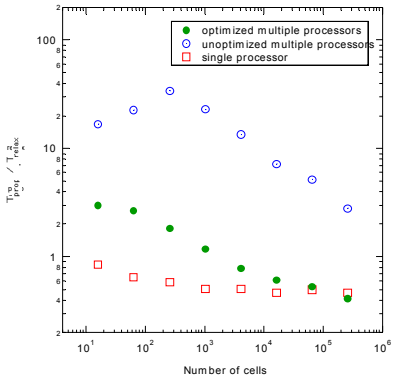

Figure 1 Importance of the inter-processor communication optimization for parallel LB. T_{relax} is the time spent in the relaxation stage that proceeds locally; T_{prop} is the time for propagation stage that is inter-processor intensive. The lower the ratio of these two, the more efficient parallelization is. With the special parceling-algorithm, the ratio was reduced by an order of magnitude so that good scaling is achievable for large enough ($N > 10^4$ where green crosses red) local system loads.

2.4. Combined RW and Lattice Boltzmann for flow propagator simulations

We combine the two distinct types of simulations as described above (particle-based RW and cell-based LB) to simulate flow-diffusion propagator. [4] First, the LB is run to yield the steady local flow velocity $\boldsymbol{v}(\boldsymbol{r})$ for each voxel. Then this is combined with the RW simulations so that the walkers, depending on its position, carry out *biased* (drifting) random walks. As the pore geometry becomes complex, the local velocity distribution widens, thus creating a formidable challenge for efficient execution of biased RWs under the complex boundary condition. Via monitoring their average auto-correlation properties such as $\langle \boldsymbol{x}(t)\, \boldsymbol{x}(0) \rangle$, we obtain the flow-diffusion propagator for a given porous medium, for which we also obtain its experimental counterpart for comparison [4], bypassing the pore-to-network-reduction step.

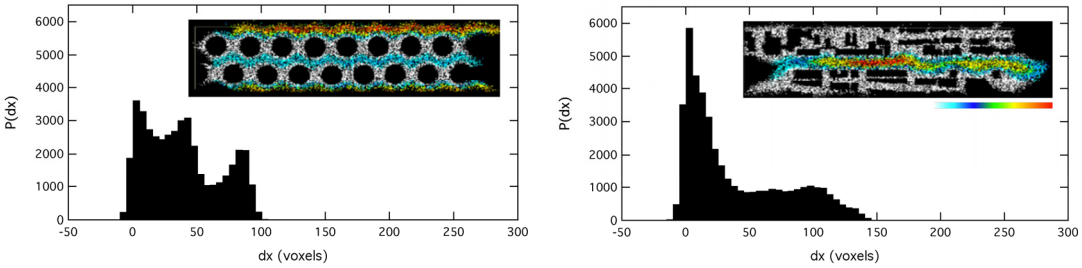

Figure 2 Probability distribution for displacement $dx = x(t)-x(0)$ in the driven flow direction of biased RWs for two qualitatively different 2D structures (analogous roughly to sandstone and carbonate rocks) after a prescribed time t after initiation of walks. The left (simple) is based on a periodic array of circular obstructions; the right (complex) is based on a part of map in Boston, MA. The color represents the local flow speed.

3. Conclusions

Combination of experiments and simulations based on the shared pore geometry provides means to clarify issues which make it difficult to extend the conventional cross-correlation methods to complex pore/fluid configurations. To gain meaningful results, it is necessary to parallelize with a robust scaling behavior, while at the same time, flexible visualization and *steering* of the process is desired for sophisticated simulation of probes. We developed a simulation technique based on *distributed objects* that alleviates the level of challenge and meets these requirements. The method is being used for a systematic, multi-pronged attack on several intractable issues for complex porous media, carbonate rocks in particular.

References

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