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SIMULATION OF FLOW AND TRANSPORT AT THE MICRO (PORE) SCALE

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ABSTRACT

An important problem in porous media involves the ability of micron and submicron-sized biological particles such as viruses or bacteria to move in groundwater systems through geologic media characterized by rock or mixed gravel, clay and sand materials. Current simulation capabilities require properly upscaled (continuum) models of colloidal filtration and adsorption to augment existing theories of fluid flow and chemical transport. Practical models typically address flow and transport behavior in aquifers over distances of 1 to 10 km where, for example, fluid momentum balance is governed by the simple Darcy's Law as a function of a pressure gradient, elevation gradient and a medium-dependent permeability parameter. In addition to fluid advection, there are multiple transport processes occurring in these systems including diffusion, dispersion and chemical interactions with solids or other aqueous chemical species. Particle transport is typically modeled in the same way as dissolved species, except that additional loss terms are incorporated to model particle filtration (physical interception), adsorption (chemical interception) and inactivation. Proper resolution of these processes at the porous medium continuum scale constitutes an important closure problem in subsurface science.

We present a new simulation capability based on enabling technologies developed for microfluidics applications to model transport of colloidal-sized particles at the microscale, with relevance to the pore scale in geophysical subsurface systems. Particulate is represented by a bead-rod polymer model and is fully-coupled to a Newtonian solvent described by Navier-Stokes. Finite differences are used to discretize the interior of the domain; a Cartesian grid embedded boundary / volume-of-fluid method is used near boundaries and interfaces. This approach to complex geometry is amenable to direct simulation on grids obtained from surface extractions of tomographic image data. Short-range interactions are included in the particle model. This capability has been previously demonstrated on polymer flow in spatially-resolved packed bed (3D) and post array (2D) systems. We also discuss the advantages of this approach for the development of high-resolution adaptive algorithms for multiscale continuum-particle and mesoscale coarse-grained molecular dynamics models.

INTRODUCTION

Numerical models of fluid flow and mass transport in porous media are widely employed in the fields of groundwater and contaminant hydrology, petroleum engineering, agricultural science, geothermal energy production, and repository science. Most subsurface simulation codes are based on mathematical models of single phase and/or multiphase flow and mass transport formulated at one or more continuum scales. In these models, geomaterials with microscale and pore scale physical and chemical heterogeneities and complex pore and/or fracture geometries are treated as homogeneous "effective media", and both fluid flow and mass transport (including mass transport mediated by colloids, nanoparticle and polymers) through these complex media are represented by averaged flow and transport equations based on concepts such as Darcy flow, relative permeability, and averaged particle transport "trapping and release rates". An important advance for current codes would be the capability of modeling particulate transport at the pore scale, and coupling this to continuum scale models as well as mesoscale models for surface chemistry. Such a capability would provide a firm scientific basis for developing

technologies for controlling the behavior of micron and submicron-sized particles of concern (radioactive and/or chemically toxic colloids, bacteria, or viruses, for example) in the subsurface, and would enable a more accurate and reliable assessment of the impact of small particles and polymers on problems such as contaminant fate and transport, and applications such as CO_2 sequestration and enhanced oil recovery.

These industrial and scientific applications require proper resolution of the biological and chemical processes at the porous medium continuum scale-specifically, discrete particulate interactions in complex microscale (pore level) geometry. The mathematical research issues include resolution and gridding of pore scale porous media geometry, coupling of an appropriate particulate representation model to the fluid dynamics, numerical accuracy and stability of the particle method, resolved interfaces for multiphase flow, upscaling techniques, and adaptive algorithms for multiscale coupling.

A non-Newtonian continuum rheology model such as a shear-thinning power law or Bingham fluid model is one approach to representing particulate matter, but more complex models are required for materials whose behavior depends on their past history. The rheology of some polymer solutions could be represented as continuum viscoelastic fluids, but these models present their own difficulties to computing solutions because of instabilities which result from the system being described with mixed mathematical formalisms, e.g., elliptic-parabolic equations [15]. In addition, the ratio between the particle size and the pore size is not always small enough to justify this approach. An appropriate particulate representation coupled to the fluid dynamics is needed to determine the behavior of polymers and colloids. An alternative approach would be to use a dissipative particle dynamics model to simulate both the polymer chains or particles and the fluid in which they are suspended or dissolved [14]. In principle a small ensemble of polymer molecules and the surrounding fluid could be simulated using classical molecular dynamics techniques. However, experience with applications such as protein folding indicates that this approach would be beyond the capabilities of petascale computing systems unless the polymer molecular weights were very small.

It is well known, however, that the essential behavior of polymers and colloidal-sized particles can be captured though coarse-grained models such as the Kramers' "bead-rod" representation [8], or the coarser Rouse "bead-spring" representation [11]. In these models the polymer is represented as discrete point masses (the beads) connected by rigid rods or entropic springs. The dynamics of polymers in solution is then modeled with a combination of stochastic (Brownian) forces and Stokes-law viscous drag forces (related through the fluctuation-dissipation theorem). Hydrodynamic coupling between the moving particles and the fluid is necessary to accurately describe these systems. In addition, biological macromolecules are chemically active, charged, and so interact through screened Coulombic interactions. These physical effects are characterized by intra-polymer, inter-polymer, and polymer-wall interaction potentials, which may be long-ranged. Because of the small time scales associated with the dynamics of small particles and macromolecule chain segments, small time steps are currently required to obtain accurate results from models that couple particle dynamics and fluid flow. New multiscale techniques for coupling are necessary to enable long time simulations of particulate transport coupled to continuum models for subsurface applications.

The meshing technique used for gridding pore scale geometry must be amenable to surface extraction from experimentally derived image data obtained from packed bed columns of porous media; and computational fluid dynamics (CFD) codes should be able to directly simulate flows on the meshes obtained from tomographic imagery without loss of geometric detail in a fast and accurate manner. Complex geometries have more traditionally been treated with conforming grids, especially in the finite element community. However, geologic media are highly irregular and dense. There are new stable and accurate approaches to gridding based on a volume of fluid representation that are specifically intended to facilitate adaptive mesh refinement and to enhance parallel scalability. This technique is also known as the embedded boundary method (EB). In this approach, the surface is represented by its intersection with an underlying rectangular grid, or a cookie-cutter approach. This leads to a natural, finite-volume discretization of the PDE on irregular control volumes adjacent to the boundary. The primary unknowns are assumed to live at the centers of the Cartesian grid control volumes, i.e., as if the boundary wasn't there. Such an approach has been shown to give consistent and stable discretizations, even in the case of moving boundaries. One of the principal advantages of the embedded boundary method is that the problem of generating the description of the geometry on the grid starting from surface tessellations produced, for example, by a CAD system has been completely solved. In addition, the volume of fluid representation is a natural description of multiphase flows with resolved interfaces. It is also complementary to a fast and accurate level-sets method for surface extraction

from image data without loss in geometric detail [5,16].

We have developed new simulation tools for modeling flow and transport of polymers at the microscale. The enabling technologies for this capability have been refined for microfluidic applications where our interest has been to extract biological species such as DNA in a fluid using channels packed with obstructions as in a packed bed or post array channel [20,17,19,10]. These flows and configurations are relevant to flow and transport of colloidal-sized particles in geophysical subsurface systems. Our approach involves coupling a micro-scale (pore level) flow model and a particle method [20,17,19,10]. The numerical stability of the entire scheme is determined by the fluid alone while also resolving particle interactions, and, thus, allowing for larger timesteps that will enable multiscale coupling and system-level modeling. The goal of this paper is to present these enabling technologies as a new alternative in subsurface simulation, and, ultimately, to demonstrate direct simulation of subsurface flow and particle transport in realistic geophysical environments, as influenced by obtained tomographic and related imagery of rock and packed bed systems. This requires a consistent and self-contained approach to algorithms and software used in numerical modeling. We achieve this through use of adaptive embedded boundary volume-of-fluid methods in the APDEC Framework developed under the DOE SciDAC program.

1 Technical Approach

We leverage enabling technologies developed for microscale flows of DNA in extraction microdevice geometries to simulate flow and transport in idealized pore scale geometries. The backbone of our approach is a projection method for incompressible viscous fluid fluids. Irregular geometry is treated with embedded boundary volume-of-fluid methods, or a "cookie-cutter" technique. Particle interactions are incorporated by applying a hierarchy of hard constraints on the system.

1.1 Equations of motion

We use the Navier-Stokes equations to model a particle-laden solvent as a continuum on domain Ω:

$$\begin{aligned} \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u} + \frac{1}{\rho}\nabla P &= \nu\Delta\mathbf{u} + \frac{1}{\rho}\mathbf{F} \\ \nabla\cdot\mathbf{u} &= 0. \end{aligned} \tag{1}$$

These equations describe an incompressible fluid of density ρ, pressure P, velocity $\mathbf{u}$, and Newtonian viscosity ν, subject to an additional body force $\mathbf{F}$. On the domain boundary $\delta\Omega$ we have the no-slip boundary condition $\mathbf{u} = 0$.

The polymer solute is represented as a collection of point masses each subject to Newton's second law of motion

$$m_\alpha \frac{d^2\mathbf{x}_\alpha}{dt^2} = m_\alpha \frac{d\mathbf{v}_\alpha}{dt} = \mathbf{f}_\alpha. \tag{2}$$

Here m_α is the mass of the α^{th} particle, $\mathbf{x}_\alpha$ is its coordinate, and $\mathbf{v}_\alpha$ is its velocity. The particle is subject to a force $\mathbf{f}_\alpha$ which combines a Stokes drag term with a stochastic (Brownian) perturbation,

$$\mathbf{f}_\alpha = m_\alpha\gamma(\mathbf{u}(\mathbf{x}_\alpha) - \mathbf{v}_\alpha) + \mathcal{F}_{\mathbf{B}\alpha}. \tag{3}$$

Here, $1/\gamma$ is a phenomenological relaxation time ($m\gamma = 6\pi\mu b$ for a Stokes sphere of radius b) , and $\mathcal{F}_{\mathbf{B}}$ is the stochastic force

$$\langle \mathcal{F}_{\mathbf{B}\alpha}(t)\rangle = 0 \tag{4}$$

$$\langle \mathcal{F}_{\mathbf{B}\alpha}(t)\mathcal{F}_{\mathbf{B}\alpha}(t')\rangle = \sigma_\alpha^2 I\delta(t-t') \tag{5}$$

$$\sigma_\alpha = \sqrt{2m_\alpha\gamma k_B T}, \tag{6}$$

with k_B being Boltzmann's constant and T the temperature.

The force $\mathbf{F}$ acting on the fluid is

$$\mathbf{F}(\mathbf{x}) = -\sum_\alpha \mathbf{f}_\alpha\delta_\epsilon(\mathbf{x}-\mathbf{x}_\alpha) \tag{7}$$

where δ_ϵ represents a smoothed Dirac delta function with length scale ϵ.

In addition to the incompressibility condition (1) we have additional constraints on the particles: (i) inter-particle spacing is constant

$$\|\mathbf{x}_\alpha - \mathbf{x}_\beta\| = a \tag{8}$$

if particles α and β represent adjacent nodes in a ball-rod polymer representation; (ii) particles cannot pass through a physical boundary,

$$\mathbf{x}_\alpha \in \Omega; \tag{9}$$

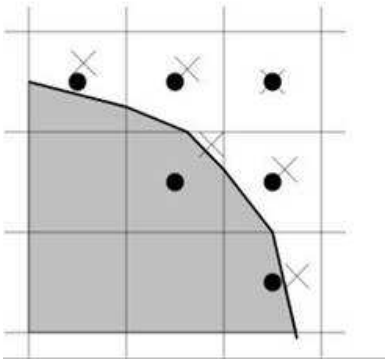

Fig. 1. Example of embedded boundary "cutting" regular cells. Solid dots are cell-centers, x's are centroids

and (iii) rods cannot cross. These constraints are applied in a hierarchical manner.

1.2 Microscale pore geometry

We use a Cartesian grid embedded boundary method to discretize the equations of motion in the presence of irregular boundaries in microenvironments. In this approach, the irregular domain is discretized as a collection of control volumes formed by the intersection of the problem domain with the cubic Cartesian grid cells (see Figure 1). The various operators are approximated using finite volume differences on the irregular control volumes, with the fluxes computed using the primary discretized dependent variables, which approximate the solution evaluated at the centers of the original Cartesian cells. This approach has been used as the basis for second-order accurate methods for elliptic, parabolic, and hyperbolic PDEs in two and three dimensions [7,9,4,13]. These methods also have been combined using the predictor-corrector approach in [3] to provide a second-order accurate projection method for the incompressible Navier-Stokes equations for problems in irregular geometries [19,2]. This is the underlying algorithm for solving the fluid equations (1,1).

The embedded boundary approach to complex geometry is compatible with a fast and accurate technique for surface extraction from CAD and image data [5,16]. In this technique fast marching level sets methods are used to obtain a surface rendering from the image . The surface is then represented on a Cartesian grid with implicit functions, making possible direct simulation in porous media with algorithms based on embedded boundaries. We have demonstrated the implicit function technique for ideal pore scale geometries in 2D and 3D. Figure 2 is an example of 2D flow in a microchannel with a structured array of posts or cylinders. Shown is the tranverse pressure gradient which is non-zero due to the geometry. Figure 3 is an example of 3D flow in a cylinder randomly packed with microspheres resembling a packed bed column. The following implicit function is used to represent the surfaces on the grid for both the 2D and 3D examples:

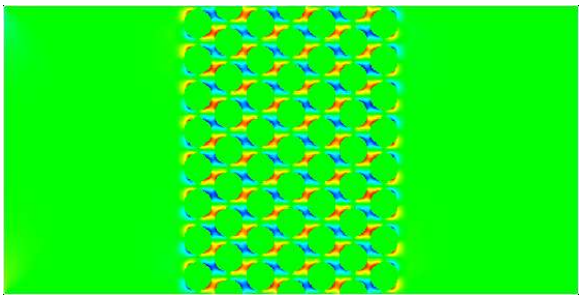

Fig. 2. 2D idealized pore geometry represented as post array microchannel. Flow is left to right. Pressure gradient in vertical direction is shown. Posts are 20μm in diameter.

$$\phi(x) = \min_k(|\vec{x} - \vec{x}_k|^2 - r_k^2) \tag{10}$$

where $\vec{x}_k$ = center of k^{th} sphere, r_k = radius of k^{th} sphere and $\vec{x} : \phi(\vec{x}) = 0$ on the boundary.

1.3 Particle interactions

Our previous versions of the particle method have included varying degrees of fidelity in particle interactions. In [20] we elastically bounced particles of surfaces but ignored the rod crossing constraint which is common in other implementations [6]; the particle timestep was two orders of magnitude less than the stable fluid timestep. In [18] we used a soft potential for rod-rod and bead-surface interactions in 2D, and explained a hard constraint algorithm with fluid coupling in [19] (see Figure 4). Currently we use a hierarchical approach to enforce the constraints of the particle system as in [10]:

1. Calculate unconstrained particle motion due to Newton's Second Law (2).
2. Calculate motion subject to rod length constraint (8).
3. Calculate motion subject to rod-rod crossing constraint (e.g., [18,19]).
4. Calculate motion subject to bead-surface crossing constraint (9).

The rod length constraint, which is similar to the molecular dynamics `SHAKE` algorithm [12], can be differentiated to obtain another constraint, on velocity, similar to molecular dynamics `RATTLE` algorithm [1]. Also, the rod-rod and bead-surface crossing constraints can be enforced simultaneously to obtain a larger timestep

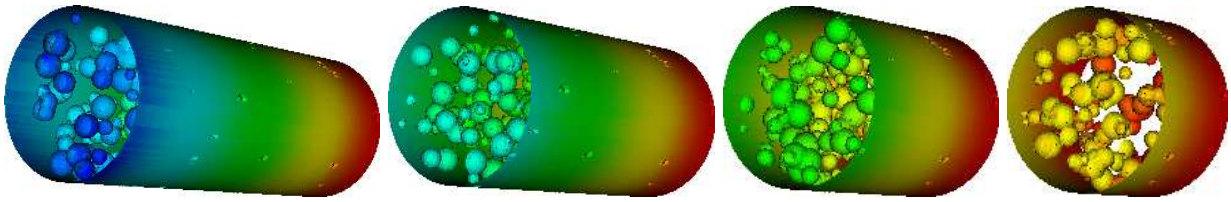

Fig. 3. 3D idealized pore geometry represented as microtube randomly packed with glass beads, with clipped views. Computed pressure is shown. Spheres range in diameter from 10 to 30μm.

on the order of a stable fluid timestep determined by advection alone (CFL condition), enabling system-level modeling [10].

CONCLUSIONS

We have explained and demonstrated how computational tools developed for microscale flows are relevant to subsurface flow and transport in porous media. For detailed results we point to our previous work on hybrid fluid-particle coupling at the microscale [20,17–19,10]. The Cartesian grid representation of irregular boundaries has several advantages over other methods. Grid generation is trivial and fast with implicit function representation on grid of surface boundaries from raw image data when compared to methods which make use of body-fitted or unstructured grids which typically smooth geometric details and are slow to grid. Also, the method results in an overall good discretization technology (e.g., finite differences on rectangular grids are stable and accurate, geometric multigrid). Next, the embedded boundary approach to solid surfaces can be extended to higher-order front tracking of material interfaces, important to resolved multiphase flow in porous media. Furthermore, direct simulation of flow and transport in realistic pore geometries is possible using level sets to shrink wrap a surface from tomographic image data. Finally, coupling to adaptive mesh refinement (AMR) is straightforward and provides a powerful tool for multiscale, multiphysics simulation.

Short range particle interactions in a fluid must be modeled to capture proper physical behavior during polymer flow and transport. Soft potentials are a robust treatment of particle interactions, but arbitrary in structure and can limit time step. A hard potential is a simple approach to capturing essential biological and chemical properties. Event-driven algorithms enable system level modeling by putting the maximum stable particle timestep on the same level as the fluid.

Our approach to pore scale modeling is intended to facilitate coupling to high-resolution Godunov-based algorithms for Darcy flow at the continuum scale through the use of adaptive mesh and algorithm refinement. Results of computations at the pore scale can be used to devise new upscaling ideas that relate microscopic processes to macroscopic properties in a continuum Darcy model such as permeability. Similarly, adaptive algorithms can be used to resolve the smaller scales where the continuum fluid description breaks down and particle-based methods are needed to represent the solvent in a flow. In this case dissipative particle dynamics or coarse-grained molecular dynamics calculations can be integrated and sampled into the larger scale algorithm for better parameterizations.

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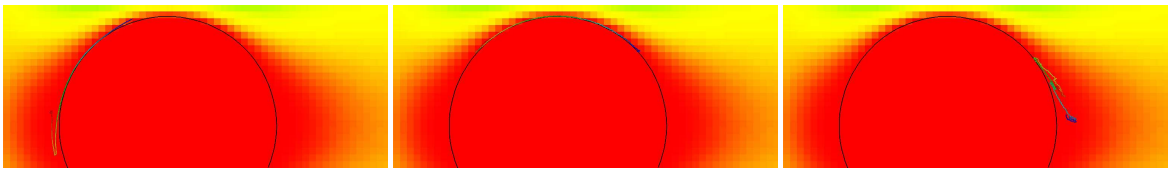

Fig. 4. Time sequence of 200-bead polymer flowing past a post in 2D demonstrating intra-polymer and polymer-structure interactions. Molecule enters from left and wraps around post in frame 1. It is slowly transported around the post close to surface where fluid velocity is nearly 0 in frame 2. Accelerated tail catches up with head in stagnation region behind post in frame 3.

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