Les Rencontres scientifiques d'IFP Energies nouvelles

Flows and mechanics in natural porous media from pore to field scale. *Pore2Field*
16-18 November 2011, IFP Energies nouvelles (France)

Numerical simulation of hydromechanical couplings by combined discrete element method and finite-volumes

Bruno Chareyre[1*], Emanuele Catalano[1], Eric Barthélémy[2]

1 Grenoble Institute of Technology, CNRS UMR 5521, 3SR lab., 11 rue des mathématiques, BP 46, 38042 St Martin d'Hères, France, e-mail : bruno.chareyre@grenoble-inp.fr
2 Grenoble Institute of Technology, CNRS UMR 5519, LEGI, 1023 rue de la piscine, 38400 St Martin d'Hères, e-mail : eric.barthelemy@grenoble-inp.fr
** Corresponding author*

Abstract — Numerical simulation of hydromechanical couplings by combined discrete element method and finite-volumes — *Discrete element modelling (DEM) enables studies of materials by modelling and analysing the phenomena that take place at the scale of their elementary components. We develop a two-phase model of saturated granular materials based on the DEM, where elasto-plastic forces arise from contact interactions. For the liquid phase, incompressible Stokes flow is considered, assuming that advective inertial forces are small compared with viscous forces. Pores geometry is defined by building a regular Delaunay triangulation of spheres, from which a system of tetrahedra (cells) arises, in a 3D framework. Finally, through the Dirichlet tessellation, the space is subdivided in polyhedra, each of them containing exactly one grain, and whose edges connect the pores. Fluid pressure is computed for each pore, and hydraulic conductivities are defined for each pore connection, accounting for the local pore-space geometry. A finite-volume formulation emerges from this approach, while some aspects are also closely related to the family of pore-network models as developped by other authors. The challenging aspect here is the determination of forces applied on particles and their integration in a dynamicaly changing skeleton geometry. The model is promising since it significantly cuts CPU time and memory footprint, compared with FEM or Lattice-Boltzman fluid models, thus enabling the modeling of representative element volumes of soils or rocks comprising thousands of particles.*

INTRODUCTION

Micro-scale measurments and modelings for heterogeneous materials has been an active area of research in the recent years. In the field of geomaterials, the discrete element methods (DEM, Cundall and Strack, 1979) has been developped for decades and is now commonly employed for studying complex aspects of the mechanical behaviour (see e.g. Scholtès 2009). It is based on the description of materials as a collection of individual particles interacting at contacts. The DEM has had great successes in the study of dry soils and rocks. The simulations of problems including a coupling with one or more intersticial fluids, on the other hand, is still a chalenging problem. We review existing approaches and we present a three-dimensional coupling model that we developed recently. Some results are presented and discussed in the last part.

1 OVERVIEW OF COUPLING METHODS

Different strategies have been adopted in the past for the solution of the fluid-solid coupling, which essentially differ in the modeling techniques adopted for the fluid part of the problem. They can be sorted in three families on this basis.

1.1 Microscale Stokes flow modeling

The numerical solution of the Stokes equations is a computationally demanding task, especially for complex three-dimensional pore geometries. Finite Element Methods (FEMs) are often used because of their flexibility in the definition of the numerical mesh. However, FEM meshes in three dimensions tend to be very large, and so are the computer memory footprint and computational times needed for the solution of the associated nonlinear system of equations. A numerical method that does not resort to the solution of large systems of nonlinear equations is the Lattice-Boltzmann

(LB) scheme. Even if LB is generally faster than the FEM, commonly implemented fixed size grids can result in considerably larger computer memory occupancy in three dimensions. Realistic microscale flow simulations in complex pore geometries generally requires access to large CPU clusters.

1.2 Continuum-discrete Darcy's flow modeling

In order to get acceptable computational costs, a number of authors have considered coarse-grid CFD methods (see e.g. Nakasa et al. 1999 for pioneering developments). In such methods, flow and solid-fluid interactions are defined with simplified semi-empirical models based on Darcy's law. There is no direct coupling at the local scale: the forces acting on the individual particles are defined as a function of mesoscale-averaged fluid velocity obtained from porosity-based estimates of the permeability. Continuum-discrete couplings succeed in making coupled problems affordable in terms of CPU cost and memory usage. The trade-off is the use of phenomenological laws for the estimation of the permeability, which limits severely the predictive power of these models in uncalibrated parameter regions. Ultimately, such strategies do not render correctly the individual particle behavior, and cannot be reliably applied to problems such as strain localization, segregating phenomena, effects of local heterogeneities in porosity, and internal erosion by transport of fines, which are all inherently heterogeneous at the micro-scale.

1.3 DEM-Pore-Network coupling

A third class of fluid flow model is the so-called pore-network modeling, based on a simplified representation of porous media as a network of pores and throats. Pore-network models have been most commonly developed to predict the permeability of materials from microstructural geometry, but have also been extended to include multiphase flow effects (see e.g. Bryant and Blunt 1992). Crucial for their success is an adequate definition of how fluids are exchanged between pores in terms of the local pore geometry. Pore-network models studies have mostly focused on flow in passive rigid solid frames. As a consequence, little attention has been devoted to the definition of forces applied to individual particles in the solid phase. This is one of the question that had to be solved for the coupling with DEM.

Early ideas for coupling pore-network flow and DEM can be found in the works of Hakuno and Tarumi (1995), and later by Bonilla (2004). The studies in this direction, however, were limited to 2D models of disc assemblies up to now. Since 2D pore geometry does not offer any free path for fluid exchanges, 2D problems imply some arbitrary definition of the local conductivity. Adapting this approach to 3D spheres assemblies, on the other hand, let us define the local hydraulic conductivity using the actual geometry of the packing, as sphere packings always define an open network of connected voids. This in turns opens up the possibility of predicting both the macro-scale permeability and the forces acting on the individual particles rather than postulating them.

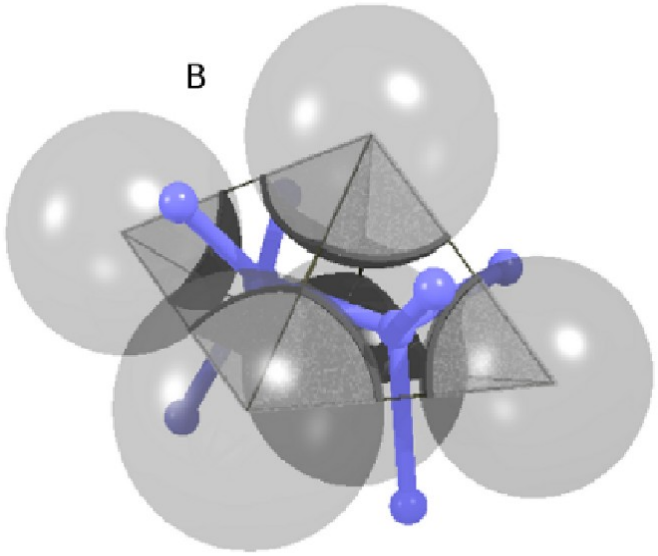

Figure 1: Regular Delaunay triangulation of spheres and it's dual (Voronoi) graph.

2 PORE-SCALE MODELING OF UNCOMPRESSIBLE STOKES FLOW IN 3D

We give here the main features of the pore-scale finite volume scheme that we developped for the coupling with DEM. For a more detailed derivation, the reader can refer to Chareyre et al. (2011). The shape of the solid particles is approximated by spheres.

A partition of the pore space in a sphere assembly can be obtained by constructing the Regular Delaunay Triangulation of the packing (Figure 2). The elementary geometrical objects emerging from this procedure are tetrahedra with spheres at each vertices, and enclosing

what we call hereafter *voids*. It is then possible to derive a finite volume formulation for Stokes flow in such mesh. The mass balance equation will link the rate of change of an element's volume to the fluxes q_{ij} exchanged between adjacent pores through facet S_{ij}:

$$\dot{V}_i^f = \sum_{j=j_1}^{j_4} \int_{S_{ij}^f} (\mathbf{u}_n - \mathbf{v}_n) ds = \sum_{j=j_1}^{j_4} q_{ij}$$

where ***u*** and ***v*** are respectively the fluid velocity and element's contour velocity. This equation links the deformation of the solid skeleton and the fluid flow via the velocity ***v***, wich is interpolated from particles velocity (i.e. motion of the vertices of the tetrahedra).

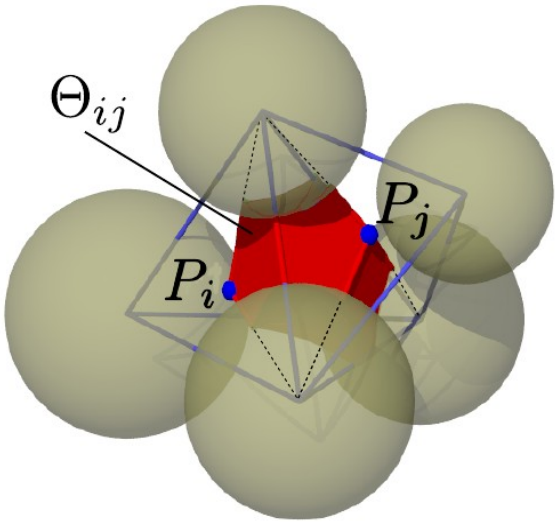

Figure 2: A throat between adjacent volume elements.

The flux q_{ij} can be expressed as a function of the pressure jump between elements *i* and *j*. We proposed to define the function by using the hydraulic radius of the throat between the two elements (Chareyre et al. 2011), the throat itself being defined by the branch that is the dual of facet S_{ij} in the Voronoi's graph (Figure 2). This finally links the deformation to the pressure field $\{p_i\}$, that we assume piecewise constant. If the conductivity of the throat is noted k_{ij} :

$$\dot{V}_i^f = \sum_{j=j_1}^{j_4} q_{ij} = k_{ij} \frac{p_i - p_j}{l_{ij}} = K_{ij}(p_i - p_j)$$

This equation gives the linear system that has to be solved at each time-step of a simulation, giving the pressure field as a function of the velocity field of the particles. The forces exerted by the fluid on each particles can finally be derived from the pressure field, with the help of momentum conservation equation. It can be decomposed in three terms which are contour integrals of the hydrostatic pressure (Archimed's force), of the piezometric pressure, and of the viscous shear stress, respectively:

$$\mathbf{F}^k = \int_{\partial\Gamma_k} \rho\Phi(\mathbf{x})\,\mathbf{n}\mathrm{d}s + \int_{\partial\Gamma_k} p\,\mathbf{n}\mathrm{d}s + \int_{\partial\Gamma_k} \tau\,\mathbf{n}\,\mathrm{d}s = \mathbf{F}^{b,k} + \mathbf{F}^{p,k} + \mathbf{F}^{v,k}$$

3 RESULTS

3.1 Permeability predictions

By generating dense sphere packings in a cube and imposing pressure at the top and bottom boundaries, it is possbile to simulate a permeameter test (Figure 3). The results show that the model is capable of predicting the permeability of sphere packings without prior calibration, as seen on Figure 4.

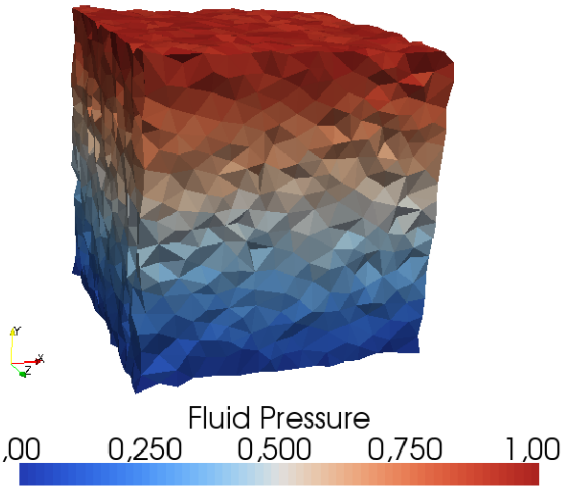

Figure 3: Pressure field in a simulated sphere packing subjected to an imposed pressure gradient for permeability test simulation.

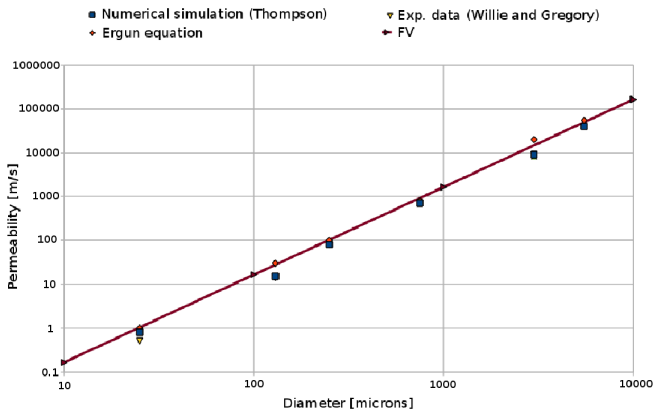

Figure 4: Permeability predictions vs. experimental measurments and analytical relations.

3.2 Time integration

This fluid flow model has been implemented in the DEM software YADE [4]. The time integration scheme has been validated by simulating the classical Terzaghi consolidation problem, where the time evolution of a drained porous material under applied stress is examined. Figure 6 shows that the results are extremely close to the closed form solution. Note that the permeability and stiffness entering the closed form solution were obtained directly from simulations, and by no means not adjusted in order to match the analytical result.

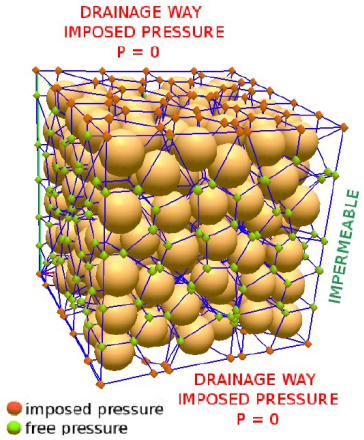

Figure 5: A typical packing used for Terzaghi's consolidation simulation.

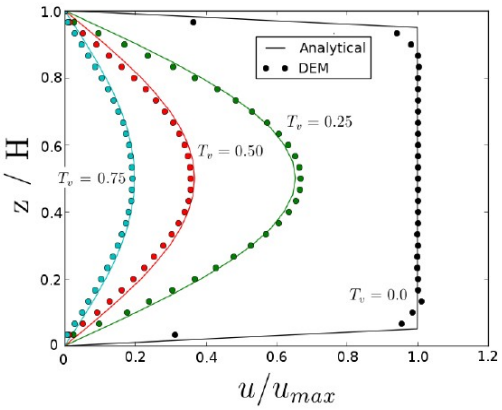

Figure 6: Evolution of normalized pressure with time in a simulated consolidation problem: result of the coupled model vs. closed form solution.

CONCLUSION

The coupling has been validated and predictive capabilities have been confirmed. We believe this approach can be extended to more complex flow equation, including compressible fluid and/or two-phase flow, and that the developments will benefit from the numerous research already done by other authors in the field of pore-network modeling. A modified version of the model with compressible fluid has already been applied successfully to the simulation of cohesive materials under high pressure. We currently focus our work on applications to internal and external erosion, transport of fines and clogging phenomena, and hydrofracturing.

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