A parallel scientific software for heterogeneous hydrogeoloy

J. Erhel [a] *, J.-R. de Dreuzy [b], A. Beaudoin [c], E. Bresciani [a], and D. Tromeur-Dervout [d]

[a]INRIA,35042 Rennes Cedex, France

[b]Geosciences Rennes, UMR CNRS 6118, France

[c]LMPG, University of Le Havre, France

[d]CDCSP, University of Lyon 1, France

1. Introduction

Numerical modelling is an important key for the management and remediation of groundwater resources. As opposed to surface water and to highly karstic geologies, groundwater does not flow in well-identified open streams but is like water flowing in the voids of a sponge. Several field experiments show that the natural geological formations are highly heterogeneous, leading to preferential flow paths and stagnant regions. Transport of contaminant by advection and dispersion induce a large spreading of the particles generally called plume. The characterization of the plume remains a much debated topic [6,9,10]. Because data give a rather scarce description of the medium hydraulic properties, predictions rely heavily on numerical modelling. Numerical modelling should integrate the multi-scale geological heterogeneity, simulate the hydraulic flow and transport phenomena and quantify uncertainty coming from the lack of data. High performance computing is necessary to carry out these large scale simulations. In this paper, we describe the scientific platform HYDROLAB, which integrates in a modular structure physical models and numerical methods for simulating flow and transport in heterogeneous porous and fractured media.

2. Physical models

2.1. Geometry and data

We consider two types of geological domains, either porous media or fractured media. Since data is lacking, the physical model of porous media is governed by a random permeability field, following a given distribution law. In order to cover a broad-range of structures, we consider finitely correlated, fractal or multifractal distribution laws. The geometry is kept very simple and is a deterministic 2D or 3D regular polyhedron. Fractured media are by nature very heterogeneous and multi-scale, so that homogenisation approaches are not relevant. In an alternative approach, called the discrete approach, flow equations are solved on the fracture network, explicitly taking into account the geometry of the fractured medium, and thus the structure of the connected network. According to recent observations of fractured rocks, fractures are characterized by a variety of shapes and a broad range of lengths. The physical model is thus based on a complex and stochastic geometry, where the geological medium (the surrounding

---

*this work was partly funded by the Grid'5000 grant from the French government

matrix) is a cube; fractures are ellipses with random distributions of eccentricity, length, position and orientation. The main feature of our model is the length distribution, which is given by a power law. We first consider an impervious matrix, because almost no water flows in it [8,5]. For some applications, it is also important to consider the coupling between the matrix and the fractures.

2.2. Governing equations

Well tests are the first source of information on the hydraulic properties of underground media. Numerical modelling of these tests involves computation of transient flow in large domains. We assume here that the medium is saturated. Flow is governed by the classical Darcy law and the mass conservation law:

$$\left\{ \begin{array}{l} v = -K\nabla h, \\ s\partial h/\partial t + \nabla . v = q \end{array} \right. \qquad (1)$$

where the Darcy velocity v and the hydraulic head h are unknown, K is a given permeability field, s is a given storativity parameter and q is a given source term. An initial condition and boundary conditions close the system. For steady-state flows, the time derivative disappears.

In order to characterize plumes of contaminant, numerical simulations consist in computing the velocity field over large spatial domains and simulating solute transport over large temporal scales [9]. We consider here one inerte solute and a steady-state flow. Governing equations are:

$$\frac{\partial(\epsilon c)}{\partial t} + \nabla.(\epsilon c V) - \nabla.(\epsilon D \nabla c) = 0 \qquad (2)$$

where ϵ is the given porosity, c is the unknown solute concentration and D is the given dynamic dispersion tensor. Boundary conditions and an initial condition complete the equation.

3. Numerical methods

The physical model is not complex in itself since equations are linear but both the broad geological heterogeneity and the lack of measures require dealing with uncertain physical and geometrical properties. Therefore, this observation underscores the need for efficient Uncertainty Quantification (UQ) methods. Moreover, the spatial and temporal dimensions are very large, in order to study multi-scale effects and asymptotic behaviour. Numerical modelling must overcome two main difficulties, memory size and runtime, in order to solve very large linear systems and to simulate over a large number of time steps. High performance computing is thus necessary to carry out these large scale simulations.

In flow computations, we use a method of lines in the case of transient equations and get a system of ODEs after spatial discretization. In both transient and steady-state cases, we choose a hybrid mixed finite element method, which computes accurately the velocity and ensures mass conservation. For porous media, the geometry is simple and the mesh is a regular grid. For fracture networks, the geometry is complex, so that it is quite difficult to generate a mesh. We have designed a two-fold mesh generator, with a preprocessing step before meshing each fracture separately [7].

At each time step, we get a large sparse symmetric positive definite linear system. Direct solvers are efficient for medium size systems but suffer from too big memory requirements for large size systems. Therefore, we prefer to use iterative solvers. Algebraic multigrid methods appear to be very efficient, either as such or as preconditioners of Conjugate Gradient method [2,3]. In transport computations, we choose a particle tracker method, because it does not introduce numerical dispersion in advection-dominated problems. We have designed a simple but efficient parallel algorithm which allows to consider large temporal domains [1].

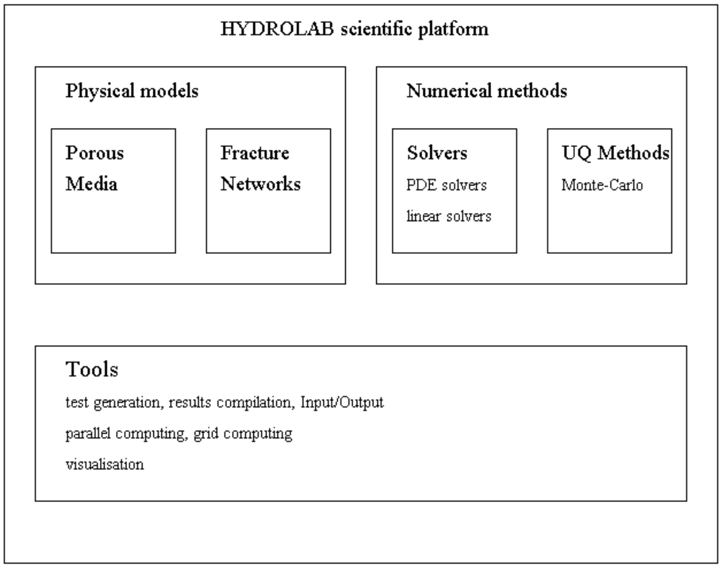

Figure 1. Software platform Hydrolab.

The permeability field is a random variable and the geometry of fracture networks is random. Hydrogeological studies aim at describing the random velocity field and the random dispersion of solute. They must rely on Uncertainty Quantification methods. Currently, we use a classical Monte-Carlo approach [7]. It is non intrusive in the sense that each sample is a deterministic simulation, using classical spatial and temporal discretizations. It is easy to implement and can be applied to any random field, either data or geometry. However, only the mean of random output can be attained with few samples; other statistical results require much more samples. Therefore, more sophisticated UQ methods can be considered, such as non intrusive spectral methods or intrusive Galerkin methods.

4. Parallel software Hydrolab

We have developed a fully parallel object-oriented software, called HYDROLAB, which provides a generic platform to run Monte-Carlo numerical simulations of flow and transport in highly heterogeneous porous media and in fracture networks. The software is organized in three main parts, respectively dedicated to physical models, numerical models and various computing tools (see Figure 1). Physical models include heterogeneous porous media and discrete fracture networks. We plan to develop a coupled model for porous fractured media. The physical model includes the generation of the random geometry and the random permeability field, the mesh generation, the spatial discretization by a mixed finite element method. The numerical methods include ODE solvers, linear solvers, multilevel methods, a particle tracker, UQ methods. The tools are for test generation, results compilation, Input/Output, visualization, geometric operations, parallel computing, grid computing, etc. This modularity allows a great flexibility and portability. The software is written in C++ and is implemented on machines with Unix, Linux or Windows systems. Graphical functions are written with OpenGL and parallel programming relies on the MPI library. The software integrates open-source libraries such as sparse linear solvers for flow computation.

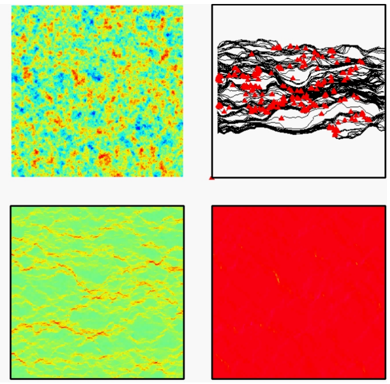

Figure 2. Simulation result for heterogeneous porous media: permeability field (top left), solute transport (top right), horizontal velocity field (bottom left), vertical velocity field (bottom right).

5. Some numerical results

We have done multiparametric Monte-Carlo simulations for solving steady-state flow and transport problems with 2D heterogeneous porous media [7]. An example of simulation output is depicted in Figure 2. We have done many experiments on a parallel cluster of the Grid'5000 computing resource installed at INRIA in Rennes and we got good performances with parallel sparse linear solvers and our parallel particle tracker. Results can be found in [4] and [1].

Thanks to our specific mesh generator, we are able to consider any random geometry of fracture networks. An example of network and simulation output is given in Figure 3. We currently solve steady-state flow problems, using Preconditioned Conjugate Gradient with a multigrid preconditioner.

6. Current and future work

We have designed a parallel modular software for solving flow and transport problems in heterogeneous and fractured geological media. Our performance results show that our software is very efficient for dealing with random 2D heterogeneous porous media. We are extending this work to 3D domains and have designed multilevel methods based on subdomain decompositions. As far as fracture networks are concerned, we are now able to generate a mesh for any network and to solve steady-state flow problems. We are doing more experiments for improving parallel performances.

Future work concern transient flow problems in porous and fractured media and transport problems in fracture networks. Also, we plan to investigate non intrusive Uncertainty Quantification methods, in order to get more statistical information than with Monte-Carlo simulations.

REFERENCES

1. A. Beaudoin, J-R. de Dreuzy, and J. Erhel. An efficient parallel particle tracker for advection-diffusion simulations in heterogeneous porous media. In *Euro-Par international conference*, 2007.
2. A. Beaudoin, J. Erhel, and J.-R. de Dreuzy. A comparison between a direct and a multigrid

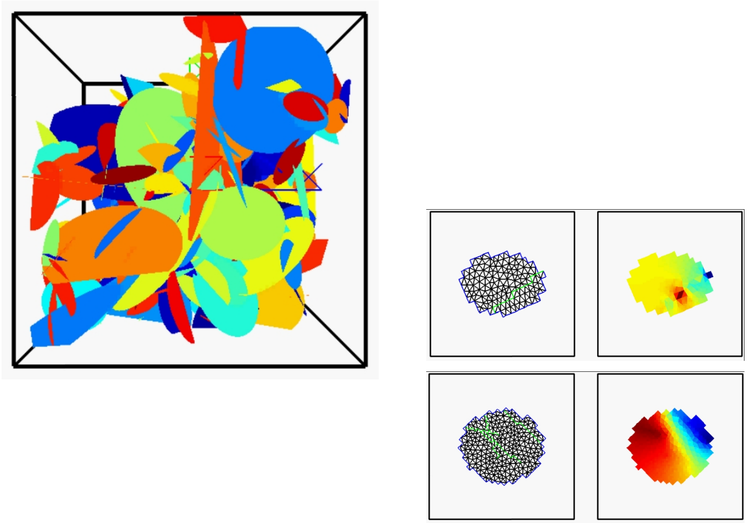

Figure 3. Simulation result for Discrete Fracture Networks: an example of fracture network (left); two fractures from the network (right) with mesh (left) and hydraulic head (right).

sparse linear solvers for highly heterogeneous flux computations. In *Eccomas CFD 2006*, volume CD, 2006.

3. A. Beaudoin, J. Erhel, and J.-R. de Dreuzy. Parallel numerical simulations for flow and transport in heterogeneous 2D porous media. Technical report, INRIA, 2007.
4. N. Bouillard, P. Montarnal, and R. Herbin. Development of numerical methods for the reactive transport of chemical species in a porous media : a nonlinear conjugate gradient method. In *Coupled problems*, ECCOMAS conference, Santorini Island, Greece, 2005.
5. C. Clauser. Permeability of crystalline rock. *Eos Trans. AGU*, 73:237–238, 1992.
6. G. Dagan, A. Fiori, and I. Jankovic. Flow and transport in highly heterogeneous formations: 1. conceptual framework and validity of first-order approximations. *Water Resources Research*, 9, 2003.
7. J.-R. de Dreuzy, A. Beaudoin, and J. Erhel. Asymptotic dispersion in 2D heterogeneous porous media determined by parallel numerical simulations. preprint, INRIA, 2007. Submitted to Water Resource Research, in revision.
8. J-R. de Dreuzy, P. Davy, and O. Bour. Hydraulic properties of two-dimensional random fracture networks following power law distributions of length and aperture. *Water Resources Research*, 38, 2002.
9. L. Gelhar. *Stochastic Subsurface Hydrology.* Engelwood Cliffs, New Jersey, 1993.
10. P. Salandin and V. Fiorotto. Solute transport in highly heterogeneous aquifers. *Water Resources Research*, 34:949–961, 1998.