DarcyTools – A Multiphysics Toolbox for Groundwater Flow and Transport Analyses

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Introduction

The Swedish Nuclear Fuel and Waste Management Company (SKB) is responsible for handling all the Swedish radioactive waste, from transport of waste and construction of storage facilities to assessment of post-closure safety (*figure 1*). To be able to handle the coupled geosphere questions from site descriptive-modelling to safety assessments, DarcyTools has been developed [1]. Focussed on hydrogeology, but based on the geology of crystalline bedrocks and coupled to hydrogeochemistry, heat, and poro-mechanics, DarcyTools implements an Equivalent Continuous Porous Media (ECPM) approach to solve the groundwater flow and radionuclide transport equations during temperate, periglacial, glacial, and submerged climate conditions in frozen, unsaturated and saturated grounds [2,3].

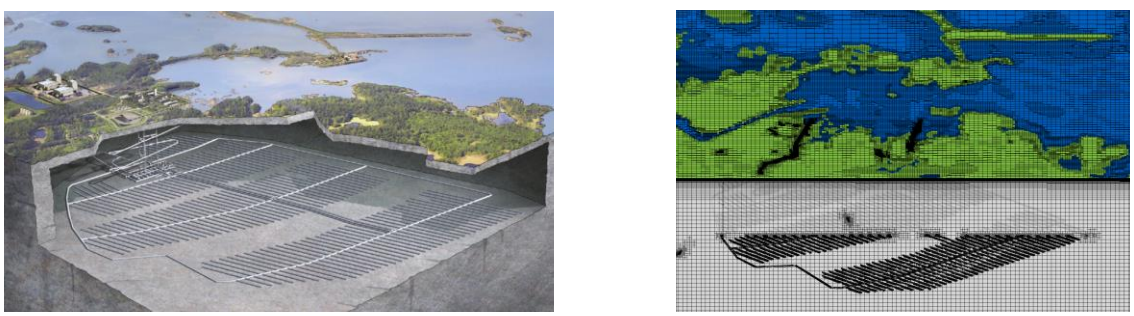

Figure 1: Partial view of a grid (right) used for Forsmark regional model (left)

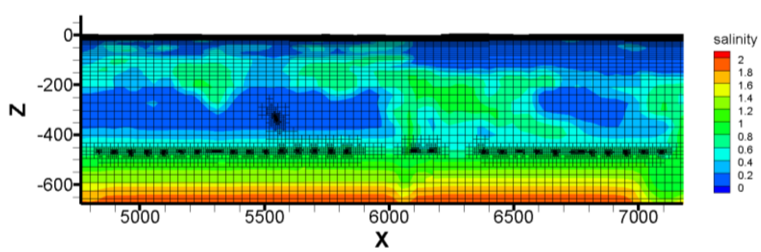

Figure 2: Example visualization of the computed salinity field before excavation of the Forsmark repository

The toolbox

The software package is optimized for engineering uses involving about 10M cells and 150M fractures, running on workstations or small clusters. It has been designed as a toolbox for solving a wide range of problems (1D, 2D, 3D, steady/transient, from μm to km, any kind of boundary conditions, arbitrary number of advection/diffusion equations, density stratification, fractured, porous, saturated/unsaturated media and more). In particular, it includes an adaptive Cartesian grid generator, a deterministic and stochastic fracture network generator, a CAD repository analysis tool (*figure 3*) and several solvers such as a Navier-Stokes solver for surface and pore-scale flows, a Darcy solver for groundwater flows, a convection-diffusion solver for heat and transport of solutes, and a mechanical solver for strain and deformation. All these solvers, including the mechanical solver, share a common finite volume kernel for an implicit discretization of the equations and a parallel multigrid preconditioned block-GMRES linear solver (MIGAL) [4] for a fast and robust convergence of the successive algebraic systems. The particle tracking is handled by an embedded Lagrangian solver implementing either a non-diffusive or a continuous time random walk method. Finally, DarcyTools also embodies a number of additional special purpose models such as a subgrid multi-rate model for diffusion and adsorption of particles and solutes in immobile water zones (*figure 2*), a permafrost model for freezing and thawing processes, a Richard's model for flow in unsaturated zones, and a grouting model for injection of non-Newtonian fluids in fractures.

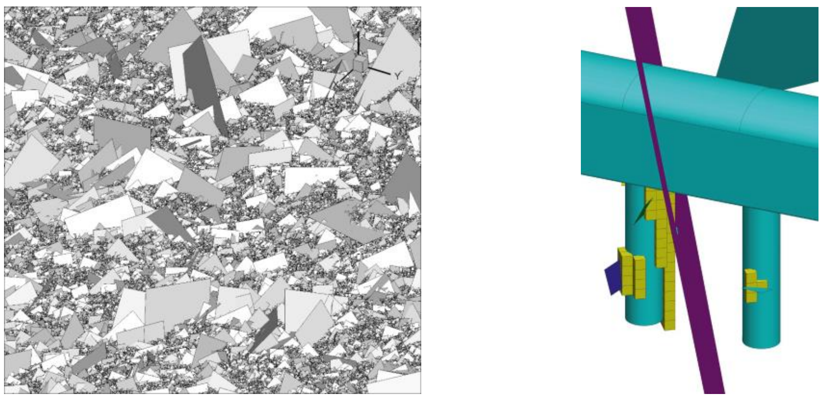

Figure 3: Partial view of a 14M fracture network in repository analysis (left) and illustration of computational cells simultaneously in contact with deposition holes and fractures (right)

Discussion

DarcyTools has been successfully applied in Safety assessment modelling in Sweden, Finland, and Taiwan during the last 15 years. We intend here, in this session, to share some of our experiences in coding and computing complex, heterogeneous, non-linear and strongly coupled problems associated with real safety assessment applications. In particular, we will address the need for slope limiters in case of sharp variation of permeability. We will discuss the importance of a conservative linearization scheme (modified Picard iteration scheme) for numerical convergence, accuracy and small time step constraints; e.g., with the latent heat term of the heat equation during phase changes. We will also explain MIGAL's technique of solving several coupled equations as one with a block-smoother when it comes to releasing the small time-steps constraints e.g. in computations of the density interface between brine and fresh water. Finally we will share our hybrid (MPI+OpenMP) parallelization experience and our usual speedups on workstations with typical linear and non-linear engineering cases.

References

[1] U. Svensson and M. Ferry, *DarcyTools: A computer Code for Hydrogeological Analysis of Nuclear Waste Repositories in Fractured Rock*, Journal of applied Mathematics and Physics, 2, 365-383, (2014).

[2] U. Svensson and S. Follin, *Groundwater Flow Modelling of the Excavation and Operational Phases - Forsmark*, SKB R-09-19, Svensk Kärnbraänslehantering AB, (2010).

[3] P. Vidstrand, S. Follin and N. Zugec, *Groundwater Flow Modelling of Periods with Periglacial an Glacial Climate Conditions - Forsmark*, SKB R-09-21, Svensk Kärnbraänslehantering AB, (2010).

[4] M. Ferry, *New Features of MIGAL Solver*, 9th International PHOENICS User Conference, Moscow, (2002).