

Documentation for the code PERFORM

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The code PERFORM (ParticleE-tracking model for Fractured pORous Media) is dedicated to simulate solute transport in heterogeneous fractured porous media.

Simulation conditions are described in the folder "Input" where the file "File_names.txt" contains the names of the parameter file (located in the folder "Param_files") and the domain file (located in the folder "Domain_files").

Parameter files

The parameter file contains the following parameters:

- domain length in the longitudinal direction (L_x)
- domain length in the transversal direction (L_y)
- matrix diffusion coefficient (D_m)
- matrix porosity (ϕ_m)
- number of particles
- transfer probability (p_{lim})
- simulation option (0/1:infinite/finite matrix)
- time step for result post-processing

It must be noticed that in the corresponding article [Roubinet *et al.*, 2012] the domain length is denoted L where $L = L_x = L_y$

Domain files

The domain file describes the segments composing the studied fracture network. The first line corresponds to the number of segments and the following lines to the description of each segment with one line per segment with the following information:

number of segments

- cartesian coordinate of the first extremity
- index of the first extremity
- cartesian coordinate of the second extremity
- index of the second extremity
- flow velocity
- segment aperture
- index of the segment
- list of the index of the neighboring segments

For extremity coordinates, the referential coordinate is assumed to be at the center of the domain and the coordinates are described as (x, y) . Extremities and segments numbering must start from 0 and the neighboring segments correspond to segments sharing one extremity with the studied one.

Examples

Examples of these previously described files are present in each of the two folders "Parameter files" and "Domain files" corresponding to the simulations presenting in the article [Roubinet *et al.*, 2012].

Files "Parameters1.txt" and "Parameters2.txt" correspond to the physical parameters used in [Roubinet *et al.*, 2012], where $D_m = 10^{-8} \text{ m}^2/\text{s}$ and $10^{-6} \text{ m}^2/\text{s}$ respectively.

Files "Domaink_fast.txt", "Domaink_medium.txt" and "Domaink_slow.txt" describe the segments of a k -division level Sierpinski lattice with the configuration *Fast*, *Medium* and *Slow flows* of Roubinet *et al.* [2012] respectively.

Libraries

The code uses the libraries CGAL-3.2.1, boost_1_49_0 and RngStream.

User has to enter the include folders of CGAL-3.2.1 and boost_1_49_0 and the library CGAL-3.2.1 (libCgal.a or Cgal.lib). The RngStream library is provided with the code in the folder "RngStream".

Comments

When running the code, user should enter the path containing the folders "Input" and "Output".

Simulation results corresponding to solute arrival times will be located in the folder "Output".

For comparison with classical results, some options must be activated:

- comparison with infinite matrix [*Tang et al.*, 1981]: the simulation option of the parameter file must be set at 0
- comparison with parallel fractures regularly spaced out [*Sudicky et al.*, 1982]: as the symmetry assumption of this latter solution is not valid for a pulse impulsion, transfer times required to reach a neighboring fractures by diffusion through the matrix must be divided by 2 to obtain similar results. That can be done by uncomment line 61 of the source file "Transfer.cpp" located in the folder "Code/src/Transport".

Citation: Roubinet D., de Dreuzay J.-R., Tartakovsky D. M., 2012. Particle-tracking simulations of anomalous transport in hierarchically fractured rocks, Computer and Geosciences.

References

Roubinet D., de Dreuzay J.-R., Tartakovsky D. M., 2012. Particle-tracking simulations of anomalous transport in hierarchically fractured rocks, Computer and Geosciences.

Sudicky, E.A., Frind, E.O., 1982. Contaminant transport in fractured porous- media - analytical solutions for a system of parallel fractures. Water Re- sources Research 18, 16341642. PT: J; TC: 276.

Tang, D.H., Frind, E.O., Sudicky, E.A., 1981. Contaminant transport in fractured porous-media - analytical solution for a single fracture. Water Resources Research 17, 555564. PT: J; TC: 317.