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A free software for pore-scale modelling: solving Stokes equation for velocity fields and permeability values in 3D pore geometries

Kirill Gerke (1), Roman Vasilyev (2,4), Siarhei Khirevich (3), Marina Karsanina (4,1), Daniel Collins (5), Dmitry Korost (2), and Dirk Mallants (1)

(1) CSIRO Land and Water, (2) Geology Faculty, Lomonosov Moscow State University, (3) KAUST, (4) Institute of Geosphere Dynamics, Institute of Physics of Earth, (5) CSIRO IM&T

In this contribution we introduce a novel free software which solves the Stokes equation to obtain velocity fields for low Reynolds-number flows within externally generated 3D pore geometries. Provided with velocity fields, one can calculate permeability for known pressure gradient boundary conditions via Darcy's equation. Finite-difference schemes of 2nd and 4th order of accuracy are used together with an artificial compressibility method to iteratively converge to a steady-state solution of Stokes' equation. This numerical approach is much faster and less computationally demanding than the majority of open-source or commercial softwares employing other algorithms (finite elements/volumes, lattice Boltzmann, etc.) The software consists of two parts: 1) a pre and post-processing graphical interface, and 2) a solver. The latter is efficiently parallelized to use any number of available cores (the speedup on 16 threads was up to 10-12 depending on hardware). Due to parallelization and memory optimization our software can be used to obtain solutions for 300x300x300 voxels geometries on modern desktop PCs. The software was successfully verified by testing it against lattice Boltzmann simulations and analytical solutions. To illustrate the software's applicability for numerous problems in Earth Sciences, a number of case studies have been developed: 1) identifying the representative elementary volume for permeability determination within a sandstone sample, 2) derivation of permeability/hydraulic conductivity values for rock and soil samples and comparing those with experimentally obtained values, 3) revealing the influence of the amount of fine-textured material such as clay on filtration properties of sandy soil.
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