Title (max 120 characters): 3D simulation of active–passive tracer dispersion in polygonal fractured geometries

Summary (max 200 words): We simulate advection–diffusion flow of tracers in fractured rock geometries. Voronoi tessellation generates polygonal patterns, which we then use to introduce fractures and obtain fractured geometry. The rock geometry is discretized using a scalable, in-house developed discretization software. Lattice-Boltzmann and random-walk particle-tracking methods are employed to obtain flow field and recover tracer behavior, respectively. Tracers are allowed to cross semi-permeable interface between fractures and matrix. In addition, tracers can have variable partitioning coefficients. The implemented numerical framework allows simulating field-scale tracer experiments designed to estimate residual oil saturation. Use of HPC platform is necessary to perform such simulations in three dimensions.

Introduction

We perform pore-scale simulations of flow and tracer dispersion in fractured porous media. Such phenomena occur, for instance, during tracer experiments performed for the estimation of residual oil saturation. Polygonal patterns may serve to generate fractured geometries (Raghavachary, 2002). In this study, we use Voronoi tessellation to create three-dimensional fractured rock geometries. In our simulations, we introduce non-zero fracture thickness, explicitly resolving fracture space. This allows mimicking both fractured polygonal patterns occurring in nature (An et. al. 2017) with sub-percent porosity, and super-permeability ("super-k") channels. The latter are specific, in particular, to the Middle East oil reservoirs, and characterized by the porosity of 10% or more (Cunningham et al. 2009).

After generating "fractures", we use in-house developed software to discretize it. We then employ the lattice-Boltzmann (LBM) and random-walk particle-tracking (RWPT) methods to simulate pore-scale 3D Stokes flow and tracer dispersion in generated geometries. With current computational facilities, such 3D simulations can only be done on high-performance computing platform. Discrete nature of both LBM and RWPT makes them a perfect fit for discrete computers, and allows performing accurate advection–diffusion simulations over multiple time scales, necessary for the complex practical problems.

Geometry generation and discretization

We use Voronoi tessellation to create fractured patterns. The idea behind this approach is i) to introduce a set of seed points in the volume of interest, and ii) to find locations around each seed point with space points closer to this seed point than to any of its neighbours (Figure 1). Hereafter, each location, also called "Voronoi volume" in 3D case, can be shrunk towards its seed point, and the released void space is considered as "fractures" (Figure 1).

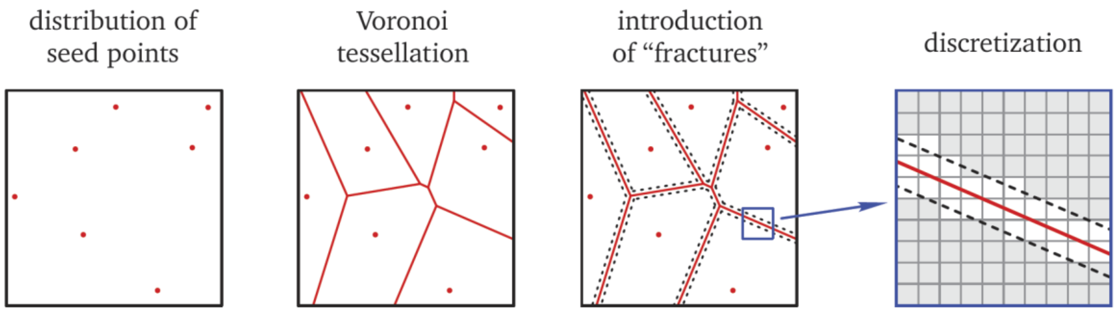

Figure 1 *Two-dimensional illustration of employed approach to generate and discretize fractured geometries. Voronoi approach is used to segment the simulation domain of interest into "rock blocks" (or matrix) and "fractures". All actual simulations are performed in three dimensions.*

Geometry discretization

Discretization of a fractured geometry can become a performance bottleneck in the simulation procedure. In this work, we implemented a parallel version of the discretization software using C language and MPI standard. We used a one-dimensional decomposition of the discrete mesh and generated "fractures" to distribute workload between MPI processes. The performance scaling of the implemented approach is shown in Figure 2. Tests were performed for random distribution of 500, 5000, and 62500 seed points resulting in 10^5, 10^6, and 10^7 "fractures", respectively. To our knowledge, maximum number of fractures to be discretized with our approach exceeds standard discrete fracture network model by a factor of 10^3.

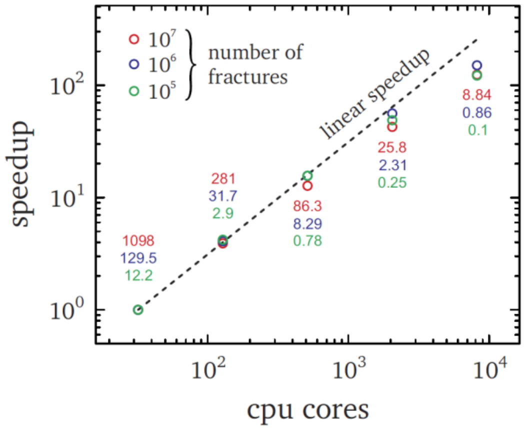

Figure 2 *Performance scaling of the code for discretization of Voronoi-tessellation based fractured geometries. Benchmarks are performed for random distribution in seed points.*

Lattice Boltzmann method

After a fractured rock geometry is generated and discretized, we calculate three-dimensional stationary flow field in its pore space. For this purpose, we employ the lattice Boltzmann method, which is a mesoscopic approach to recover fluid flow behaviour. The method operates with fluxes of fictitious particles moving along discrete set of lattice links and colliding on its nodes. The method operates solely with discrete quantities (space, time, directions of lattice links) and therefore well-suitable for high-performance computing. We use so-called two-relaxation-times version of the lattice-Boltzmann collision operator (Ginzburg et al. 2008). It can be considered as an optimal choice for Stokes flow simulations (Khirevich et al. 2015).

Random-walk particle-tracking method

The discretized geometry and the corresponding flow field are used as inputs for tracer dispersion simulations. We use the random-walk particle-tracking method (RWPT) to recover time-dependent behaviour of tracers, which are subject to advection and diffusion. After distribution of tracers in fracture space, each tracer is displaced on each iteration as follows:

$$\Delta r = r(t+\Delta t) - r(t) = v(r)\Delta t + \xi\sqrt{2D_{\mathrm{region}}\big(r(t)\big)\Delta t}$$

where r is tracer coordinate, Δt is the time step, ξ is a vector calculated from normal distribution. Velocity components $v(r)$ are obtained from LBM velocity field using zero-order approximation. D_{region} is the diffusion coefficient of a tracer located at a voxel of a region type, which can be `matrix` or `fracture`. Our RWPT implementation allows introducing semi-permeable interface between two region types. The region `matrix` has no flow components, but is assumed to consist of water, oil, and rock mass (Figure 3a). The region `fracture` is occupied solely by water and a tracer in this region is subject to advection and diffusion. While crossing the matrix-fracture interface, the probability of an accepted jump is the following (Daneyko et al., 2015, Bechtold et al. 2011):

$$\begin{cases} P_{\mathrm{f}\to\mathrm{m}} = K'\phi_{\mathrm{m}}\sqrt{D_{\mathrm{m}}/D_{\mathrm{f}}} \text{ and } P_{\mathrm{m}\to\mathrm{f}} = 1 \text{ if } K'\phi_{\mathrm{m}}\sqrt{D_{\mathrm{m}}/D_{\mathrm{f}}} < 1, \\ P_{\mathrm{m}\to\mathrm{f}} = (K'\phi_{\mathrm{m}}\sqrt{D_{\mathrm{m}}/D_{\mathrm{f}}})^{-1} \text{ and } P_{\mathrm{m}\to\mathrm{f}} = 1 \text{ otherwise.} \end{cases}$$

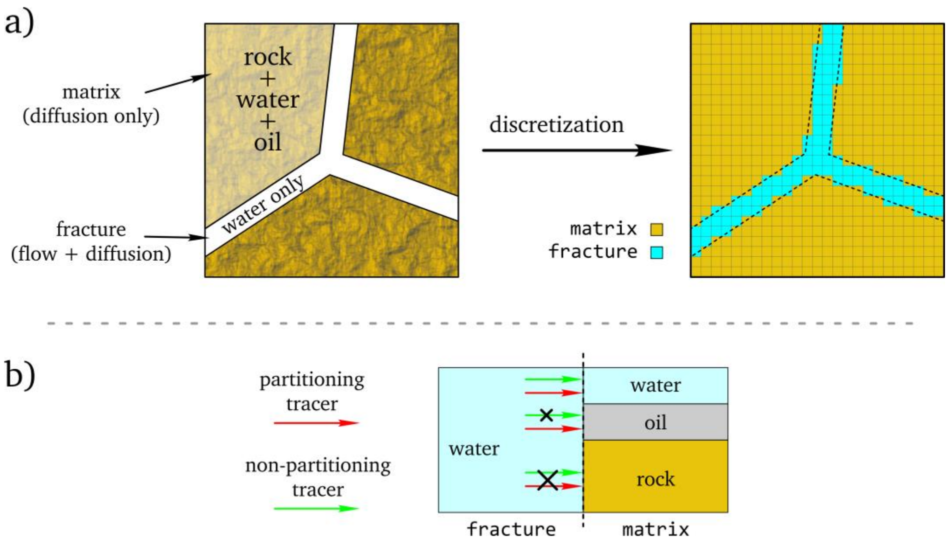

Figure 3 *a) Illustration of pore-scale and effective medium approaches used in simulations. b) Accepted and rejected jumps of partitioning and non-partitioning tracers; their probability is controlled by matrix porosity, saturations of oil and water, and by partitioning coefficient K.*

Here $P_{\mathrm{f}\to\mathrm{m}}$ ($P_{\mathrm{m}\to\mathrm{f}}$) is the probability of a tracer to jump from `fracture` to `matrix` (`matrix` to `fracture`), D_{m} (D_{f}) is the diffusion coefficient in `matrix` (`fracture`) region. ϕ_{m} denotes matrix porosity.

The quantity K' is defined as $K' = S_{\mathrm{w}} + KS_{\mathrm{o}}$, with S_w and S_o are water and oil saturations. K denotes the partitioning (or distribution) coefficient, and is defined as $K = C_{\mathrm{o}}/C_{\mathrm{w}}$, or the ratio of equilibrium concentrations of tracers in oil and water phases. Partitioning or non-partitioning tracer types can be implemented using probability of acceptance of their jumps to cross the interface between two region types (Figure 3b).
Our approach allows to have discontinuity in diffusion coefficient (i.e., between D_{m} and D_{f}). This aspect is implemented using non-linear time-splitting scheme:

$$\Delta r^*_{\mathrm{f}\to\mathrm{m}} = \Delta r_{\mathrm{f}} + \Delta r_{\mathrm{m}}\sqrt{D_{\mathrm{m}}/D_{\mathrm{f}}}\,,$$

where $\Delta r^*_{\mathrm{f}\to\mathrm{m}}$ is the corrected jump after entering `matrix` region from `fracture`, Δr_{f} (Δr_{m}) is the part of a tracer jump in `fracture` (`matrix`) regions. For the jump in opposite direction, $\Delta r_{\mathrm{m}\to\mathrm{f}}$, the similar correction is applied.

Choice of a boundary condition (or rule) for a tracer crossing the interface between `fracture` and `matrix` is a non-trivial task: its inappropriate choice can significantly degrade accuracy of the 3D concentration field (Szymczak and Ladd, 2003). In our simulations we use specular reflection boundary condition, which is more difficult to program but it provides correct distribution of tracer concentration compared to alternative boundary conditions.

First results

One of our goals is to simulate field-scale tracer experiments (Sanni et al. 2016). For this purpose, we generate a three-dimensional fractured geometry using $3 \times 3 \times 256$ seed points resulting in 2304 Voronoi blocks. Fracture porosity equals 4.6%. We discretize it with 256 lattice nodes per (average Voronoi volume)$^{1/3}$ or average edge length, l. This choice results in a “fracture” aperture of 5.6 voxels and discrete mesh of $768 \times 768 \times 65536$ voxels (Figure 4). Considering physical edge length of $l =$ 0.5m, simulations require about 10^{10} time steps to resolve time scales of a field-scale experiment. When using 20000 tracers, this translates to about 10^{15} random numbers. Efficient parallel implementation of all simulation steps (geometry generation, discretization, LBM and RWPT simulations) allowed to perform the described simulations using 2048 cpu cores.

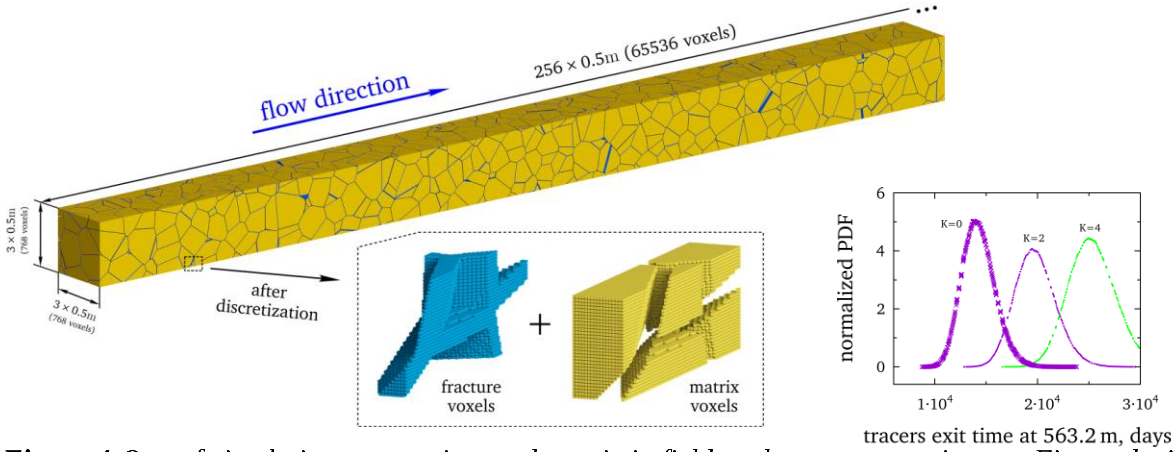

Figure 4 *One of simulation geometries used to mimic field-scale tracer experiments. Figure depicts about 20% length of the actual geometry.*

Conclusions

We use Voronoi tessellation to generate fractured patterns in three dimensions. The generated geometry is discretized with an in-house parallel discretization software. The resulting mesh is used as input for lattice-Boltzmann and random-walk particle-tracking methods to simulate advection–diffusion behavior of (non-)partitioning tracers. Efficient parallel implementation of all simulation steps allows mimicking and studying field-scale tracer experiments.

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