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Tri Dat Ngo, André Fourno, Benoit Noetinger. Modeling of transport processes through large-scale discrete fracture networks using conforming meshes and open-source software. 2018. hal-01702755

HAL Id: hal-01702755

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Preprint submitted on 7 Feb 2018

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Modeling of transport processes through large-scale discrete fracture networks using conforming meshes and open-source software

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Abstract

Most industrial and field studies of transport processes in Discrete Fracture Networks (DFNs) involve strong simplifying assumptions, especially at the meshing stage. High-accuracy simulations are therefore required for validating these simplified models and their domain of validity. The present paper proposes an efficient workflow based on open-source software to obtain transport simulations. High-quality computational meshes for DFNs are first generated using the conforming meshing approach FraC. Then, a tracer transport model implemented in the open-source code DuMux is used for simulating tracer transport driven by the advection-dispersion equation. We adopt the box method, a vertex-centered finite volume scheme for spatial discretization, which ensures concentration continuity and mass conservation at intersections between fractures. Numerical results on simple networks for validation purposes and on complex realistic DFNs are presented. An a-posteriori convergence study of the discretization method shows an order of convergence $O(h)$ for tracer concentration with h the mesh size.

Keywords: DFN, Conforming mesh, Transport processes, Vertex-centered finite volume method

1. Introduction

During recent decades, modeling of transport processes in fractured porous media has received increasing attention from the geoscientist community because of its wide range of applications in geothermal energy (Aquilina et al., 1998), petroleum exploration and production (Bourbiaux, 2010), CO₂ geological storage and nuclear waste disposal (Grenier et al., 2005; Fournon et al., 2007). Fracture networks might consist of pre-existing natural or pressure-induced fractures in the case of hydraulic fracturing (Delorme et al., 2016). Solute transport in fractured media should be studied using either continuous (Svensson, 2001; Karimi-Fard et al., 2006; Fournon et al., 2013) or discrete models (Erhel et al., 2009; Hyman et al., 2014; Berrone et al., 2017). When fractures are densely distributed and the length of fractures is of the same order of magnitude, continuous models can be used safely, because there is a representative elementary volume (REV) (Long et al., 1982; Neuman, 1988). At scales larger than the REV, the contribution of fractures may be captured in equivalent parameters that are obtained via upscaling processes (Karimi-Fard et al., 2006; Matthai and

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13 Nick, 2009; Jourdain et al., 2014). On the other hand, for sparsely distributed fracture networks, possibly
14 no REV exists; the solute is carried along connected preferential pathways of high permeability. In that
15 situation, in order to capture the effects related to the fracture sparseness, the domain should be modeled by
16 discrete approaches. The basic idea is to keep an explicit representation of fracture networks. In this work,
17 we focus on solute transport in discrete fracture networks (DFNs) assuming that flow only occurs through
18 fracture planes, the matrix surrounding fractures is disregarded.

19 Fractures are generally considered as lower-dimensional objects, i.e. 1D or 2D objects embedded in a
20 3D domain. Pipe-network approaches, which are based on the assumption of flow channeling within DFNs,
21 model fractures as 1D-in-3D objects. With this strong topological simplification, pipe-network models allow
22 to significantly reduce the computational cost for large-scale reservoirs. The accuracy of such models has
23 been investigated for steady-state flow and transport (Cacas et al., 1990; Dershowitz and Fidelibus, 1999;
24 Gylling et al., 1999). Noetinger and Jarrige (2012) recently proposed a quasi steady-state method for solving
25 transient Darcy flow in complex 3D fractured networks only. This work is then extended for accounting
26 for transfers arising from the matrix (Noetinger, 2015). At the lowest order of approximation, this method
27 needs only one unknown that is assigned at each identified intersection location between fractures. The pipe
28 network model is then recovered. Nevertheless, further studies should focus on validation of the pipe-models
29 for transient flow and transport.

30 Another simplifying assumption is to consider fractures as planar objects. High-accuracy simulations of
31 flow and transport within DFNs can be obtained on conforming or non-conforming meshes. By using non-
32 conforming meshes, advanced numerical approaches, such as the PDE-constrained optimization approach
33 (Berrone et al., 2013; Benedetto et al., 2014, 2016; Berrone et al., 2017) and the Mortar method (Erhel et al.,
34 2009; Pichot et al., 2010, 2012), allow to alleviate the meshing-related difficulties. Nevertheless, applying
35 such a method may lead to a high additional computational effort and requires adaptations of classical
36 numerical schemes to non-conforming meshes. Therefore, although creating high-quality conforming meshes
37 for such networks is a non-trivial task due to geometrical complexities, it is still being dealt with by many
38 recent studies (Hyman et al., 2014, 2015; Huang et al., 2016; Fournon et al., 2016).

39 Hyman et al. (2014) developed the feature rejection algorithm for meshing (FRAM) to generate three-
40 dimensional conforming grids for DFNs. This approach is based on constraining generations of DFNs to
41 exclude arbitrarily small features from the network, only features greater than a user-prescribed minimum
42 length scale h will be generated. Nonetheless, by removing small fractures accuracy of simulations can be
43 affected due to the loss of fracture connectivity within the resulting mesh. Huang et al. (2016) and Fournon
44 et al. (2016) recently proposed a simple yet efficient meshing approach for DFNs, the so-called "Fracture
45 Cut Method for Meshing" (FraC). The main idea of the approach is to decompose each fracture into a set
46 of connected closed contours, between which common segments will be discretized in a conforming manner.
47 Even tiny fractures are taken into account to conserve the DFN connectivity, and a strategy for moving or
48 adding intersecting points is applied to ensure an acceptable quality of the final mesh.

49 Furthermore, the resulting conforming meshes obtained from these meshing approaches have often a
 50 complex "non-manifold" topology (Sander et al., 2015). Handling such a situation usually requires the
 51 introduction of additional data fields and logic with respect to standard manifold grids. Some finite element
 52 codes using Mixed and Hybrid Finite Element Methods (MHFEM), for instance Cast3M (2017) (Fourno
 53 et al., 2016), allow to avoid this extra implementation effort. On the other hand, standard finite volume
 54 codes often only allow for manifold topologies that are predominant in realistic applications and do not
 55 address non-manifold issues. Currently, there are few finite volume simulators for subsurface flow and
 56 transport, e.g. PFLOTRAN (Lichtner et al., 2013; Hammond et al., 2014) and DuMux (Flemisch et al.,
 57 2011), able to deal with non-manifold topologies. Resulting meshes from the FRAM method were used
 58 to obtain single-phase flow solutions using PFLOTRAN, followed by Lagrangian-based particle transport
 59 modeling (Hyman et al., 2014; Makedonska et al., 2015; Karra et al., 2015; Hyman et al., 2015). The
 60 objective of this paper is to describe an efficient workflow that provides high-accuracy solute transport
 61 simulations using conforming meshes. The proposed workflow uses the FraC approach for meshing and
 62 DuMux for simulation frameworks in order to profit from its Euclidean-based transport modeling capability.
 63 It is noteworthy that other advanced conformal mesh generators such as dfnGen (Hyman et al., 2014) could
 64 be employed for the network generation and meshing, the FraC approach was chosen simply because of
 65 its user-friendliness. The workflow is able to handle with non-trivial DFN configurations, which remain a
 66 major challenge for classical methods. Furthermore, the numerical framework can easily be extended to
 67 consider multiphase, multi-component flow, transient single-phase flow or reactive transport as well as other
 68 hydrological modelling issues using DFN models.

69 The contribution is organized as follows. Section 2 provides the mathematical formulation and numerical
 70 methods for transport processes using the DuMux (Flemisch et al., 2011) code. Section 3 is focused on the
 71 methodology of the FraC approach used to obtain conforming meshes for DFNs. Numerical results of solute
 72 transport on simple and complex DFNs are shown in Section 4, both for model validation and demonstration
 73 purposes. For validation purpose, solutions of solute transport obtained with DuMux on a simple single-
 74 fracture DFN are compared to analytical solutions. Another validation on a more complex 7-fracture DFN is
 75 also proposed using numerical results from Ahmed et al. (2015) as reference. The second part of the section
 76 is dedicated to case studies of transport processes on a synthetic benchmark 33-fracture network and on a
 77 complex and realistic DFN in order to assess the reliability of the approach. Finally, we conclude the paper
 78 in Section 5 by giving some directions for further studies.

79 2. Mathematical formulation and numerical methods

80 The motion of a non-reactive solute in the subsurface can be described by the advection-diffusion equation,
 81 (Bear et al., 2012) as follows:

$$\omega \frac{\partial C}{\partial t} = \nabla \cdot (\bar{D} \cdot \nabla C - C \mathbf{v}) + q, \quad (1)$$

82 where $\omega (-)$, \overline{D} (L^2/T) are the porosity and the dispersion coefficient tensor for the solute in water, respec-
 83 tively. C (M/L^3) stands here for the solute concentration, \mathbf{v} (L/T) for the velocity field and q ($M/(L^3.T)$)
 84 for the external sink and/or source term. The velocity field \mathbf{v} is given by the Darcy’s law:

$$\mathbf{v} = -\frac{\overline{K}}{\mu}(\nabla p + \rho \mathbf{g}), \quad (2)$$

85 in which p ($M/(L.T^2)$) denotes the water pressure, \mathbf{g} the gravity acceleration vector, \overline{K} (L^2) the perme-
 86 ability tensor, μ ($M/(L.T)$) the dynamic viscosity of water and ρ (M/L^3) is its density. The water flow is
 87 assumed to be in the steady-state, therefore Equation (1) can be recast as:

$$\omega \frac{\partial C}{\partial t} = \overline{D} \nabla^2 C - \mathbf{v} \cdot \nabla C + q. \quad (3)$$

88 The one-dimensional form of Equation (3) reads as follows

$$\omega \frac{\partial C}{\partial t} = D_L \frac{\partial^2 C}{\partial x^2} - v \cdot \frac{\partial C}{\partial x} + q. \quad (4)$$

89 Although several physical models available in DuMux allow to study a wide range of subsurface problems,
 90 spanning from single-phase single-component isothermal to three-phase three-component non-isothermal
 91 flow, non-reactive solute transport is however not implemented in the code. Fortunately, there is the `1p2c`
 92 model simulating single-phase flow of a compressible fluid consisting of two components where the fluid
 93 properties such as the density and the viscosity depend upon the pressure. The primary variables of the
 94 `1p2c` model are the pressure p and the mole or mass fraction of dissolved components x^k . Basing on this
 95 model, transport processes can be simulated in DuMux with a slight modification of the code, in which
 96 the pressure-dependency of the fluid properties is removed. The steady-state fluid flow are considered, i.e.
 97 \mathbf{v} is constant, therefore, the continuity equation of the `1p2c` model becomes the advection-diffusion equation.

98
 99 The non-manifold issue of the mesh topology is solved in DuMux (2017) via the DUNE grid manager
 100 `DUNE::FoamGrid` (Sander et al., 2015). A vertex-centered finite volume scheme, also known as the *box*
 101 *method* (BM) (see, for example, Huber and Helmig (2000)), is chosen for solving flow and transport in
 102 porous media. Concretely, the computational domain \mathcal{T}_h is discretized by a finite element grid, the so-called
 103 ”primary mesh”, where h is the mesh size. Since fractures are considered as surface objects, the unit cell could
 104 be either triangles or quadrilaterals. A ”secondary mesh” which describes the finite volumes is constructed
 105 based on the finite element grid. A finite volume \mathcal{B}_i , also known as a *box*, is obtained by connecting the
 106 gravity center of element i with associated edge midpoints (see Figure 1). Thus, each finite volume is associ-
 107 ated with a node of the primary mesh. Furthermore, the model variables are defined for control-volumes but
 108 not finite elements, they are thus assigned to the grid nodes. Moreover, local physical properties of porous
 109 media, such as permeability and porosity, are specified element-wise, the corresponding values assigned to

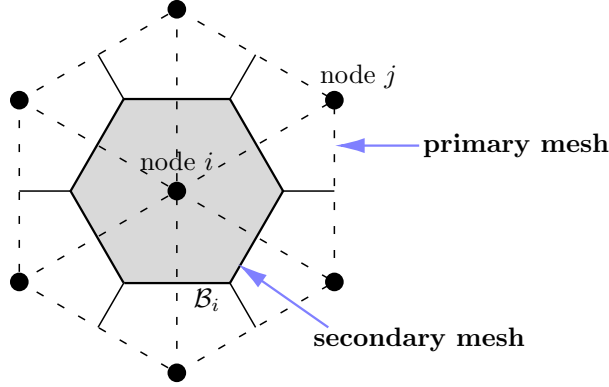


Figure 1: Spatial discretization of the box method including two meshes: "primary mesh" in dashed lines and "secondary mesh" in continuous lines. The gray polygon represents the box \mathcal{B}_i corresponding to the node i .

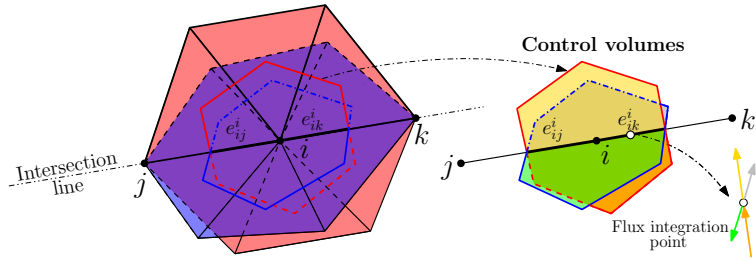


Figure 2: Illustration of the flux distribution for intersecting control volumes. The orange and yellow polygons belong to the red fracture, and the green and gray polygons belong to blue fracture. In this example, inflow occurs from the orange polygon and outflow occurs through the remaining polygons. This figure is reproduced from Hyman et al. (2015); Makedonska et al. (2015). We refer to the online version of the paper for the colors mentioned in this caption.

110 each control volume are determined by a weighted average of the properties of the sub-control volumes.

111

112 The BM inherits advantages from both the finite element and finite volume method: the finite ele-
 113 ment property makes it possible to deal with unstructured grids and the finite volume method ensures
 114 mass conservation. In addition, for flow and transport simulations on non-manifold conforming meshes,
 115 the BM unconditionally guarantees pressure continuity and mass conservation at the intersections between
 116 planar surfaces. Assume that we are considering two intersecting fractures (the red and blue ones) as in
 117 Figure 2. Since the mesh is conforming along the intersection line, the control volumes associated to the
 118 node i within each fracture share common edges (e_{ij}^i and e_{ij}^i) of the sub-control volumes, on which the
 119 fluxes are computed. Then, mass conservation at the fracture intersection can naturally be ensured, and
 120 the box method is therefore chosen as discretization method for the following flow and transport simulations.

121

122 Moreover, although the temporal discretization may be done using an explicit or an implicit Euler scheme

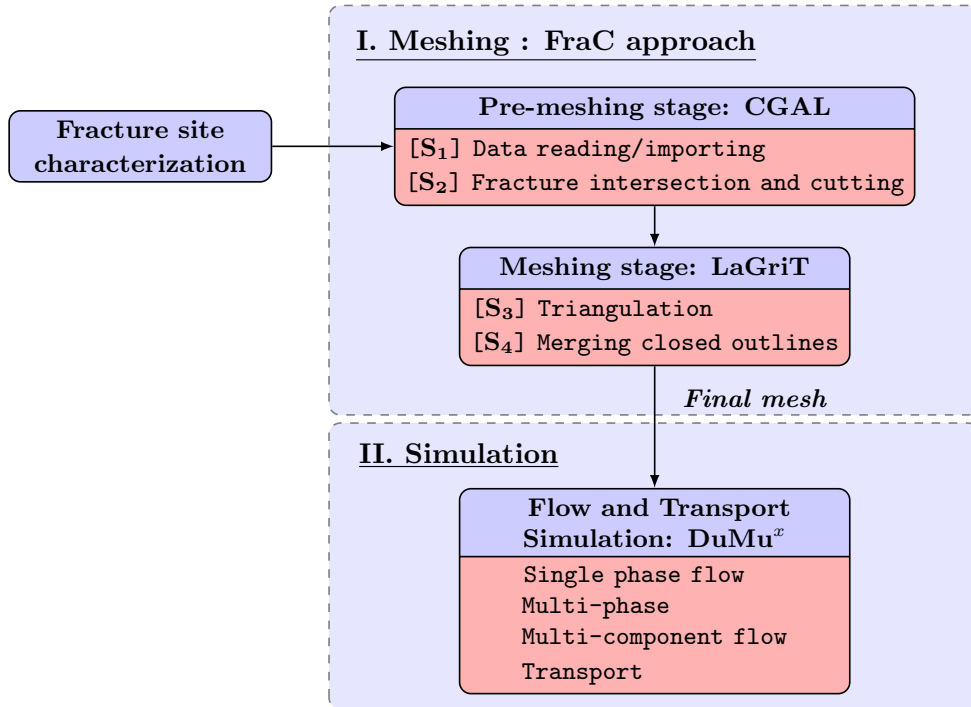


Figure 3: General flow chart from 3D mesh generation of DFNs basing on geological input datasets to numerical simulations of flow and transport processes. The framework consists of two major parts: (I) Mesh generation using the FraC approach and (II) Numerical simulations in DuMux. For the first part, the implementation of the FraC approach is carried out by using CGAL and LaGriT for pre-meshing and meshing stage, respectively. Detailed steps of each stage are also listed.

123 in DuMux, only implicit models are retained in our applications. The time-step size is controlled in an adap-
 124 tive manner based on the number of iterations needed for the Newton’s method to converge for the last time
 125 integration (Flemisch et al., 2011).

126

127 3. Mesh generation

128 3.1. Description of the meshing method

129 The FraC method involves two primary stages, i.e. pre-meshing and meshing stages (see Figure 3. The
 130 pre-meshing stage includes two steps that are all implemented using the Computational Geometry Algo-
 131 rithms Library (CGAL): (i) data reading/ importing (S_1); (ii) fracture intersections and cutting (S_2). The
 132 triangulation (S_3) and merging closed contours (S_4) processes gather together in the meshing stage, which
 133 is done by using Los Alamos Grid Toolbox (2013) because CGAL is unfortunately not able to store non-
 134 manifold data. The main features in each stage can be summarized as follows.

135

136 (i) S_1 : *Data reading/importing*

137 The input for FraC comes generally from fractured site characterizations that provide distributions of
 138 fracture forms, orientations, dimensions, and spatial locations. Fractures are then representatively approx-
 139 imated by concave polygons. Each polygon \mathcal{F}_i will then be discretized with a user-defined characteristic
 140 length h_i , that is subsequently used as the target edge length for \mathcal{F}_i in the meshing stage. It means that the
 141 edge length of the mesh triangles is of the same order of magnitude as h_i . Hence, resolution of the final mesh
 142 can be easily controlled by adjusting h_i ; high values of h_i result in coarse meshes and reducing h_i yields
 143 mesh refinement. The characteristic length h_i is fairly similar to the minimum length scale in the FRAM
 144 approach (Hyman et al., 2014, 2015).

145
 146 (ii) S_2 : *Fracture intersection and cutting*

147 The next step involves finding intersections between the polygons associated with the fractures. An octree-
 148 like approach (Khvoenkova and Delorme, 2011; Hyman et al., 2014) is used to optimize the localization of
 149 fractures in the space. More precisely, an axis-aligned minimum bounding box BB_i is created around \mathcal{F}_i
 150 where BB_i is defined by the minimal and maximal value of the corresponding coordinate of the polygon
 151 vertices. Then a preliminary test is performed to check intersection between the bounding boxes BB_i and
 152 BB_j of two fractures \mathcal{F}_i and \mathcal{F}_j respectively. The number of intersection tests between bounding boxes
 153 performed for each fracture can be reduced using a three-dimensional octree structure based on fracture
 154 locations in the corridor. This approach works well if the size of the fractures is almost of the same order of
 155 magnitude.

156 If BB_i and BB_j are not touching in space, obviously \mathcal{F}_i and \mathcal{F}_j do not intersect. Otherwise, if BB_i and
 157 BB_j intersect, the intersection test between \mathcal{F}_i and \mathcal{F}_j is then performed. The intersection line \mathcal{L}_{ij} between
 158 the \mathcal{F}_i and \mathcal{F}_j planes is first determined. Let $\partial\mathcal{F}_\alpha$ be the boundary of \mathcal{F}_α with $\alpha \in \{i, j\}$, then finding
 159 intersections between the fractures becomes finding intersections between $\partial\mathcal{F}_i$, $\partial\mathcal{F}_j$ with \mathcal{L}_{ij} . We denote
 160 $n_{ij}^{(\alpha)}$ the number of intersection points between $\partial\mathcal{F}_\alpha$ with \mathcal{L}_{ij} . So far, two cases can occur:

161 - $n_{ij}^{(i)} = 0$ or $n_{ij}^{(j)} = 0$: The fractures do not intersect.

162 - $n_{ij}^{(i)}, n_{ij}^{(j)} > 0$: In most cases, four intersection points $\mathbf{p}_i^{(1)}, \mathbf{p}_i^{(2)}, \mathbf{p}_j^{(1)}, \mathbf{p}_j^{(2)}$ ($n_{ij}^{(i)} = n_{ij}^{(j)} = 2$) may be
 163 found, where $\mathbf{p}_i^{(1,2)}$ lie on \mathcal{F}_i and $\mathbf{p}_j^{(1,2)}$ lie on \mathcal{F}_j . Degenerated cases of tangent fractures where $n_{ij}^{(i)}$ or
 164 $n_{ij}^{(j)}$ or both of them equal to one may also exist. The intersection points are then sorted to find out
 165 endpoints. Let $\bar{\mathcal{I}}_{ij}$ be the segment connecting two endpoints, \mathcal{I}_i be the portion of $\bar{\mathcal{I}}_{ij}$ which lies only
 166 on \mathcal{F}_i but not on \mathcal{F}_j , \mathcal{I}_j be the portion which lies only on \mathcal{F}_j but not on \mathcal{F}_i , and \mathcal{I}_{ij} be the portion
 167 which lies on both \mathcal{F}_i and \mathcal{F}_j (see Figure 4). Finally, the fractures intersect only if $\mathcal{I}_{ij} \neq \emptyset$.

168 The fracture cutting step expresses the key idea of the FraC approach, it is solely applied for intersecting
 169 fractures. Each of two intersecting fractures \mathcal{F}_i and \mathcal{F}_j will then be cut along the extended intersection
 170 $\bar{\mathcal{I}}_{ij}$ to obtain interconnected closed contours, subsequently referred to as "sub-fractures". To guarantee the

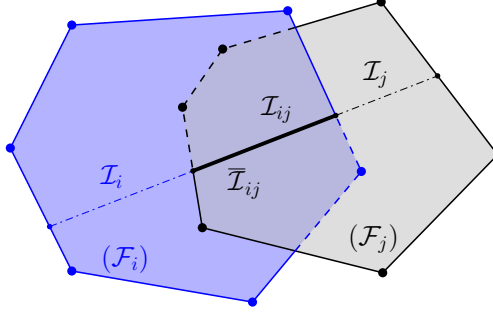


Figure 4: An example of two intersecting fractures \mathcal{F}_i (blue) and \mathcal{F}_j (gray). The extended intersection $\bar{\mathcal{I}}_{ij}$ (bold line) between them involves \mathcal{I}_{ij} (bold line), \mathcal{I}_i and \mathcal{I}_j (dashed lines).

171 homogeneity of the final mesh, the sub-fractures and more precisely, the segment $\bar{\mathcal{I}}_{ij}$ should also be dis-
 172 cretized according to the mesh characteristic length of the original fracture. For that, special focus is put
 173 on $\bar{\mathcal{I}}_{ij}$ which is also sub-divided in a homogeneous or adaptive manner. In the first case we define the target
 174 edge length $h_{ij} = \min(h_i, h_j)$ common for $\bar{\mathcal{I}}_{ij}$ and its sub-segment including $\mathcal{I}_i, \mathcal{I}_j, \mathcal{I}_{ij}$. Here, h_i and h_j
 175 are the target edge length of \mathcal{F}_i and \mathcal{F}_j respectively. In the second case, only \mathcal{I}_{ij} will be discretized with
 176 h_{ij} , the target edge length for \mathcal{I}_i and \mathcal{I}_j remains h_i and h_j respectively. At the endpoints of $\mathcal{I}_i, \mathcal{I}_j$ and \mathcal{I}_{ij} ,
 177 two strategies are flexibly applied: depending on neighborhood area, discretization points of $\partial\mathcal{F}_\alpha$ are either
 178 moved (Type I) or created (Type II) to model the intersection points (Figure 5a). These strategies allow
 179 avoiding too short edges resulting in grid cells with extremely high aspect ratio in the final mesh.

180

181 Once all edges of sub-fractures are discretized, new intersection tests between them and other fractures/
 182 sub-fractures are carried out. By a series of cutting steps, the original fractures are decomposed into a large
 183 number of connected closed contours (Figure 5b) that will be used as input for the triangulation step S_3 .
 184 The main benefit of series of cutting steps is that multiple-intersection issues vanish. For example, a prob-
 185 lem of triple intersections between three fractures $\mathcal{F}_i, \mathcal{F}_j, \mathcal{F}_k$, is transformed to standard problems of finding
 186 intersections between \mathcal{F}_k and the sub-fractures of \mathcal{F}_i and \mathcal{F}_j . The drawback of this strategy is that it in-
 187 creases the number of intersection tests and, consequently, the computational time. The consequence of this
 188 feature of the method is however beyond the scope of the present paper and will be addressed in another work.

189

190 (iii) S_3 : *Triangulation*

191 In this step, each sub-fracture will be meshed according to its own target edge length h_i (Figure 5c).
 192 LaGriT uses a conforming Delaunay triangulation algorithm to ensure that the line of intersection between
 193 any two sub-fractures is preserved. More details can be found in Murphy et al. (2001) or Hyman et al. (2014).

194

195 (iv) S_4 : *Merging meshed sub-fractures and post-treatment*

196 This step bridges the gap between the meshing part and the simulation part of our workflow. All resulting

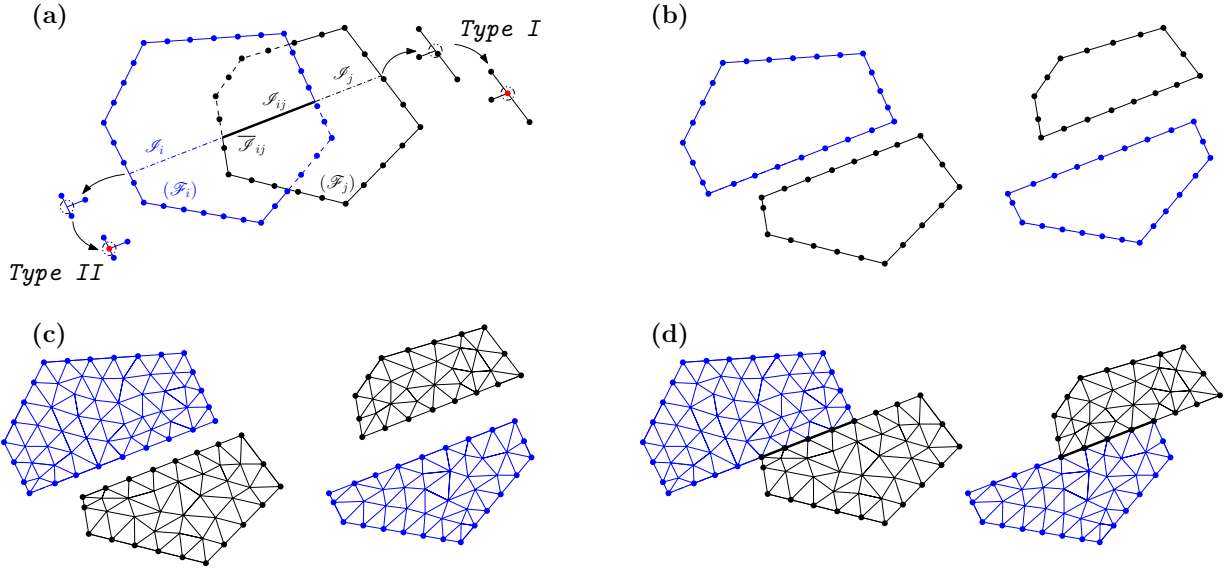


Figure 5: Illustration of the meshing steps: step S_1 – fracture intersection (a) and fracture cutting (b); step S_3 – polygon triangulation (c); and step S_4 – merging meshed polygon (d).

197 meshed closed contours from step S_3 will be merged into a single triangulation data structure, in which there
 198 will probably be duplicate vertices along the intersection lines (Figure 5d). These duplicates are detected
 199 and removed, resulting in a final fully connected mesh, that can be saved to **.inp* files which can be read by
 200 the AVS graphics program, both in binary or ASCII format. A mesh conversion of **.inp* files to **.dof* file
 201 (DUNE Grid Format, DGF) is then required to make output mesh files compatible with the DuMux code.
 202 A detailed description of the DGF and its utilization can be found on the homepage of DUNE.

203 3.2. Meshing examples

204 In this section, two applications of the FraC approach for meshing complex DFNs will be shown. The first
 205 example is a benchmark DFN, which has also been used by many previous studies (Khvoenkova and Delorme,
 206 2011; Fournon et al., 2016), and the second one is a semi-synthetic DFN where the network’s properties are
 207 closely based on the geological data from the fictional but realistic Bloemendaal reservoir (Verscheure et al.,
 208 2012).

209 3.2.1. Benchmark 33-fracture DFN (DFN_1)

210 The benchmark fracture network contains 33 disc-shaped fractures inside a $3\text{ m} \times 3\text{ m} \times 3\text{ m}$ cube.
 211 A common characteristic length h is set for all fractures. Several meshing realizations are performed with
 212 decreasing h to obtain a set of meshes with different degrees of refinement. Concretely h ranges from
 213 $9.6 \times 10^{-1}\text{ m}$ to $3.75 \times 10^{-3}\text{ m}$ resulting in meshes that contains from 2×10^3 to 8.0×10^6 grid cells. In
 214 Figure 6, we show, as an example, the DFN mesh generated by FraC with two values of h : a coarse grid

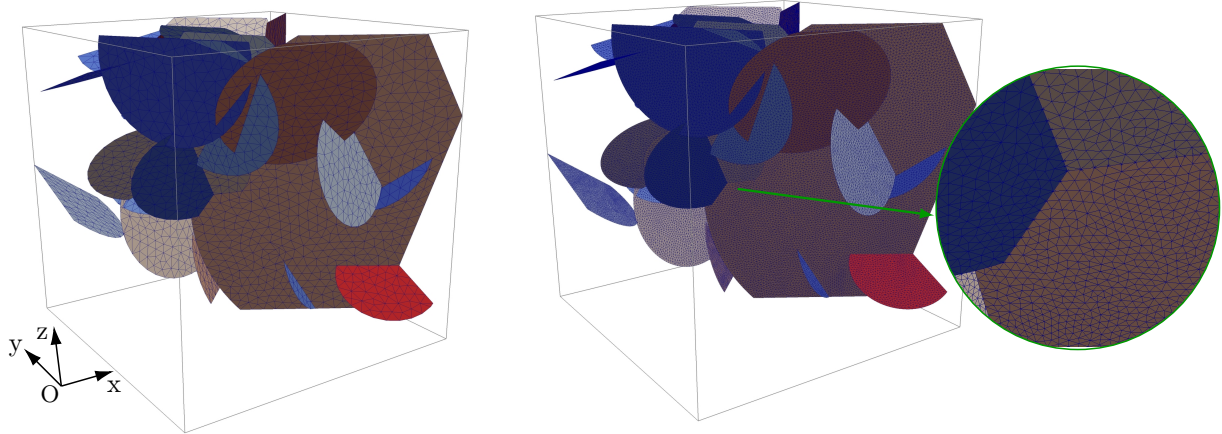


Figure 6: Two meshes of the benchmark DFN: a coarse mesh DFN_{1a} corresponding to $h_{1a} = 0.12$ m (left) and a fine mesh DFN_{1b} corresponding to $h_{1b} = 0.03$ m (right). The inset displays an example of multiple-intersection showing the mesh conformity.

215 DFN_{1a} corresponding to $h = 0.12$ m (left) and a fine grid DFN_{1b} corresponding to $h = 0.03$ m (right). This
 216 shows the ability of our code to generate not only extremely fine meshes but also very coarse meshes of the
 217 DFN while preserving the fracture network topology. The inset in this figure exhibits the mesh conformity
 218 at a multiple-intersection location.

219 3.2.2. Semi-synthetic DFN of the Bloemendaal reservoir (DFN_2)

220 The semi-synthetic DFN consists of more than 50,000 rectangular-shaped fractures that lie on a domain
 221 of $12 \text{ km} \times 15 \text{ km} \times 1.4 \text{ km}$. The flowing zone depth of the reservoir is about 200 m (Figures 7a and 7b).
 222 We use the algorithm of the FracFlow code (Beicip-FranLab, 2017) to generate the fracture network that
 223 includes two principal fracture sets: one set primarily oriented along the x -axis (red fractures, Figure 7a)
 224 with an average fracture spacing of 10.0 m and another primarily oriented along the y -axis (blue fractures,
 225 Figure 7a) with an average fracture spacing of 7.5 m. For the above colors, we refer the reader to the online
 226 version of the paper.

227 In practice, simulations using the DFN concept rarely model the whole fracture network of the reservoir.
 228 For example, in the oil field, the most common tests based on DFN conceptual models, such as well-tests,
 229 flow-meters or interference tests, consider the influence zone of a few kilometers around the wells (Bourbiaux
 230 et al., 2002). Therefore, in this case we focus solely on a part of the semi-synthetic DFN: only fractures inside
 231 a bounding box of $L_0 \times L_0 \times 1.4 \text{ km}$ (red box, Figure 7b) are taken into account, with L_0 initially equal to
 232 1 km; the DFN contains around 5×10^2 fractures. An example of resulting mesh is illustrated in Figure 7c.
 233 We then expand the DFN by increasing L_0 to ten kilometers. The number of fractures and consequently the
 234 intersections between them inside the DFN are thus increased. Figure 7d plots a log-log graph of the variation
 235 of fracture number N in the DFN bounding box with respect to the box width L_0 , showing the relationship
 236 $N \sim L_0^2$. The unit mesh size h remains constant for all meshing realizations resulting in progressively larger

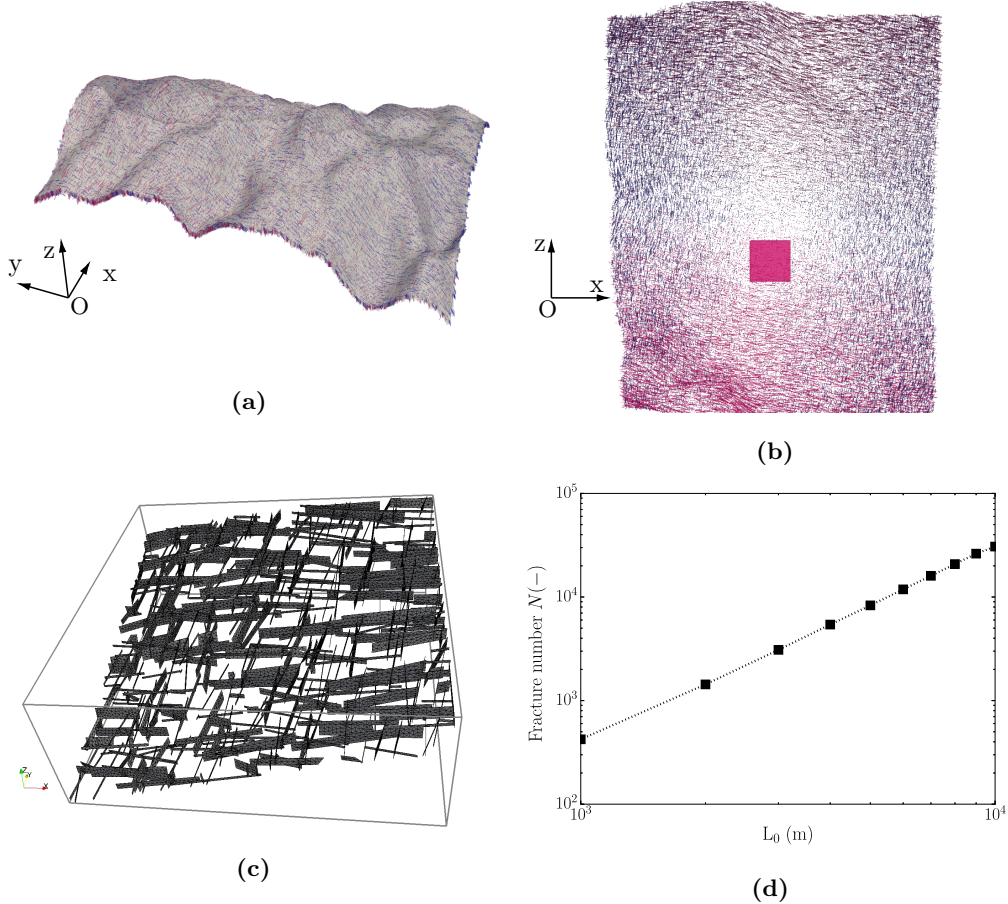


Figure 7: Semi-synthetic DFN: entire fracture network in lateral view (a) and in top-down view (b). The red box in (b) indicates a part of the DFN that is being meshed. An example of resulting mesh for the case $L_0 = 1$ km where the DFN contains around 5×10^2 fractures is shown in (c), and (d) reports the variation of the fracture number in the bounding box (in red) w.r.t. the box size.

237 grids.

238 4. Numerical results

239 In this section, numerical results are presented to evaluate the ability of DuMux to simulate solute
 240 transport in DFNs with increasing levels of topological complexity. Three validation tests are carried-out:
 241 (i) numerical solutions of solute transport in a single inclined fracture are compared to analytical solutions
 242 from Ogata and Banks (1961); (ii) validation is performed by comparing Dumux’s simulation results to those
 243 obtained by Ahmed et al. (2015) on a simple fracture network consisting of 7 interconnected fractures; and (iii)
 244 the convergence assessment of flow and transport solutions on 33-fracture DFN meshes with increasing mesh
 245 refinement. More realistic simulations are then performed on the semi-synthetic DFN of the Bloemendaal
 246 reservoir.

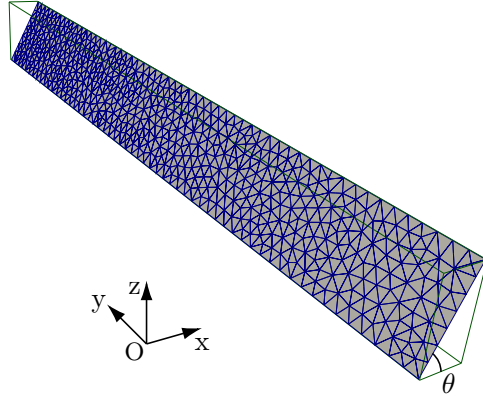


Figure 8: A snapshot of the mesh for a single inclined planar fracture embedded in 3D domain with $h = 0.4\text{m}$. The green rectangular cuboid indicates the bounding box around the fracture.

247 For simplicity, the DFNs in all examples are assumed to be homogeneous with a constant fracture aperture
 248 of $b = 10\text{ mm}$ for Example 3 and $b = 1\text{ mm}$ for the others. An isotropic permeability for all fractures $K = 10^3$
 249 mD is applied for Example 2 to be consistent with that of Ahmed et al. (2015) while, for other cases, the
 250 fractures are assigned a scalar permeability tensor $K = 10^4\text{ mD}$. The fluid viscosity is constant and equals
 251 $\mu = 10^{-3}\text{ Pa}\cdot\text{s}$.

252 4.1. Example 1: Single inclined fracture

253 The single fracture is an inclined planar rectangle of length 20 m (along the y -axis) and of width $\sqrt{5}\text{ m}$.
 254 The angle θ between the fracture normal vector and the z -axis satisfies $\tan\theta = 2$.

A concentration $C(t = 0) = 0$ is applied throughout the entire domain as initial condition. Flow occurs along the y -axis by adopting a pressure gradient $\Delta P = 10^8\text{ Pa}$ along the y -direction. Tracer is continuously injected into the domain with an imposed concentration C_0 (relative concentration $C' = C/C_0 = 1$), the prescribed boundary conditions are summarized as follows:

$$\begin{cases} C = C_0 \text{ on } y = 0 \text{ m,} \\ C = 0 \text{ on } y = 20 \text{ m,} \\ \Phi = 0 \text{ otherwise.} \end{cases} \quad (5)$$

255 The transport analytical solution of this problem is given by Ogata and Banks (1961):

$$C(x, t) = \frac{C_0}{2} \left[\operatorname{erfc} \left(\frac{x - vt}{2\sqrt{D_L t}} \right) + \exp \left(\frac{vx}{D_L} \right) \operatorname{erfc} \left(\frac{x + vt}{2\sqrt{D_L t}} \right) \right] \quad (6)$$

256 where C_0 is the imposed concentration on the inlet and erfc is the complementary error function. When
 257 the ratio vx/D_L (i.e. the Péclet number Pe) is large enough, the second term in equation (6) is negligibly

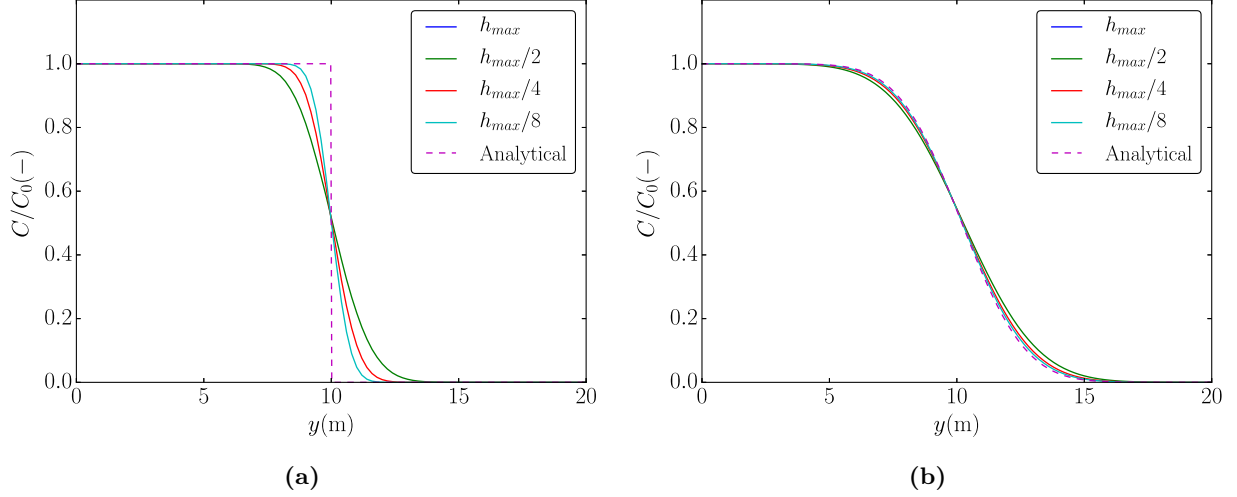


Figure 9: Concentration profile for the test case of continuous injection of tracer within a single fracture at $t = 2 \times 10^4$ (s): (a) $v_1 = 5 \times 10^{-4} \text{ m.s}^{-1}$, $D_1 = 1 \times 10^{-9} \text{ m}^2.\text{s}^{-1}$ ($Pe_1 = 10^7$), and (b) $v_2 = 5 \times 10^{-4} \text{ m.s}^{-1}$, $D_2 = 1 \times 10^{-4} \text{ m}^2.\text{s}^{-1}$ ($Pe_2 = 10^2$). Mesh size of the coarsest mesh $h_{max} = 0.4\text{m}$. Discontinuous line on (a) represents the approximate solution from Equation (7) while the one on (b) illustrates the exact solution from Equation (6).

258 small and often disregarded (Ogata and Banks, 1961; Bodin et al., 2007), one obtains the approximate
 259 solution as follows:

$$C(x, t) = \frac{C_0}{2} \operatorname{erfc} \left(\frac{x - vt}{2\sqrt{D_L t}} \right). \quad (7)$$

260 According to Ogata and Banks (1961), only a maximum error of less than 3% between the exact and
 261 approximate solutions in Equations (6) and (7) is shown for $Pe > 500$.

262

263 Different meshes are used to model this problem with h decreasing from $h_{max} = 0.4\text{m}$, the mesh size of
 264 the coarsest mesh, to $h = h_{max}/8$. Figure 8 shows a mesh example of the fracture for $h = 0.4\text{m}$. Two cases
 265 according to two dispersion coefficient values are studied. We consider in the first case a convection-dominant
 266 process with a low dispersion coefficient $D_1 = 1 \times 10^{-9} \text{ m}^2.\text{s}^{-1}$ and the mean fluid velocity $v = 5 \times 10^{-4}$
 267 m.s^{-1} resulting in a Péclet number $Pe_1 = L \times v/D_1 = 10^7$. In the second case, v remains unchanged but
 268 the dispersion coefficient is increased up to $D_2 = 1 \times 10^{-4} \text{ m}^2.\text{s}^{-1}$, the corresponding Péclet number is thus
 269 equal to $Pe_2 = 10^2$.

270

271 Figure 9 depicts concentration profiles obtained from numerical simulations on different meshes with
 272 variable h for both cases at $t = 2 \times 10^4$ (s). Analytical solutions from Equation (7) for $Pe_1 = 10^7 \gg 500$ and
 273 from Equation (6) for $Pe_2 = 10^2 < 500$ are also illustrated. In the first case, there are offset between the
 274 analytical and numerical curves mainly at the front location (around $y = 10$ m). This discrepancy is possibly
 275 caused by both the error of the approximation in Equation (7) and numerical diffusion effects. It can be
 noted that, when the grid is refined, the numerical curves tend to the analytical solution. The numerical

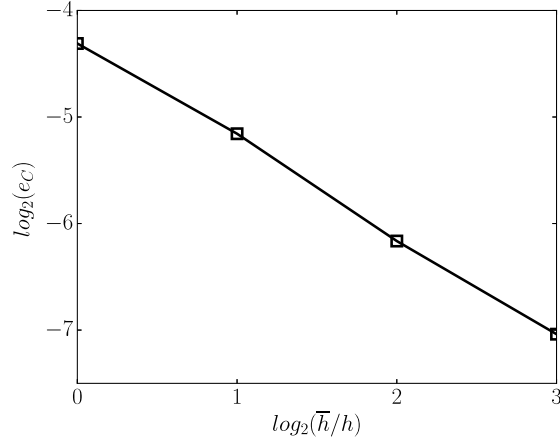


Figure 10: Log2-plot of the discrete concentration L^2 errors for the case $D_2 = 1 \times 10^{-4} \text{ m}^2.\text{s}^{-1}$ showing an order of convergence $O(h)$ for the concentration.

276 diffusion effect vanishes for the second case when the physical diffusion effect is stronger. Numerical solutions,
 277 particularly for the solution on the finest mesh, i.e. $h = h_{max}/8 = 0.05 \text{ m}$, are in perfect agreement with the
 278 analytical one.

The exact solution from the second case $D_2 = 1 \times 10^{-4} \text{ m}^2.\text{s}^{-1}$ is now used for convergence study. Indeed, to estimate the BM convergence order, a L^2 norm of tracer concentration error e_C is defined as:

$$e_C = \left(\frac{\sum_{\mathcal{B}_i \in \mathcal{T}_h} |\mathcal{B}_i| \times (C_{ex, \mathcal{B}_i} - C_{\mathcal{B}_i})^2}{\sum_{\mathcal{B}_i \in \mathcal{T}_h} |\mathcal{B}_i| \times C_{ex, \mathcal{B}_i}^2} \right)^{\frac{1}{2}}. \quad (8)$$

279 Here, $C_{\mathcal{B}_i}$ and C_{ex, \mathcal{B}_i} stand for the discrete and analytical concentration solution of the box \mathcal{B}_i respectively
 280 while $|\mathcal{B}_i|$ denotes the box area.

For $k \geq 2$, the convergence order $col2(k)$ of the L^2 norm of the error on the solution between grid level k and $k - 1$ can be evaluated as:

$$col2(k) = \frac{\log(e_C(k)/e_C(k-1))}{\log(h(k)/h(k-1))}. \quad (9)$$

281 Figure 10 displays the convergence rate for the concentration of the box method, showing an order of
 282 convergence of $O(h)$.

283 4.2. Example 2: 7-fracture DFN

284 In this benchmark exercise, solutions of DuMux are compared to those from Ahmed et al. (2015), who
 285 use the cell-centred control-volume distributed multi-point flux approximation (CVD-MPFA) approach as
 286 discretization method. The studied DFN lies inside a $200 \times 150 \times 15 \text{ m}^3$ system. For validation purposes,
 287 simulation on 2D model from Ahmed et al. (2015) is chosen as a reference. Our mesh (Figure 11a) has the
 288 same resolution as that used by Ahmed et al. (2015) (figure 11b). The conforming Delaunay mesh generated
 289 by the FraC approach contains 4554 grid cells while the Ahmed's mesh contains 4662 triangular cells.

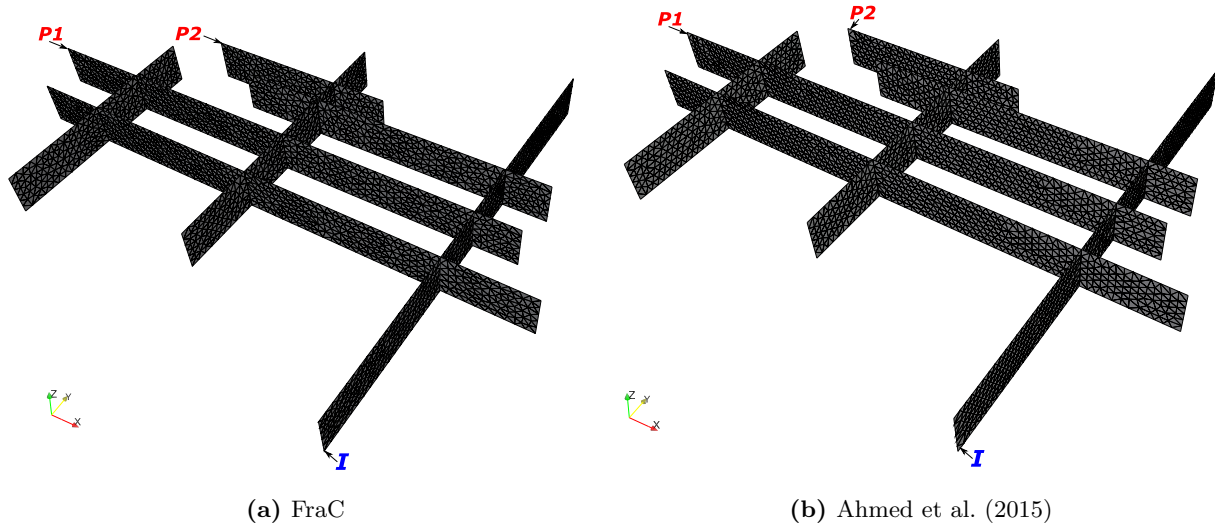


Figure 11: 7-fracture DFN: mesh generated using FraC approach (a) and that used in Ahmed et al. (2015) (b).

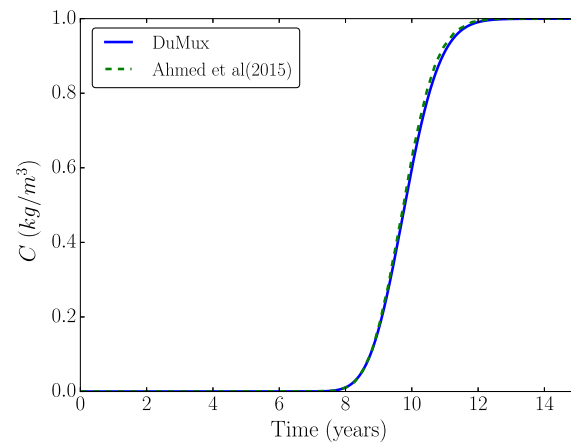
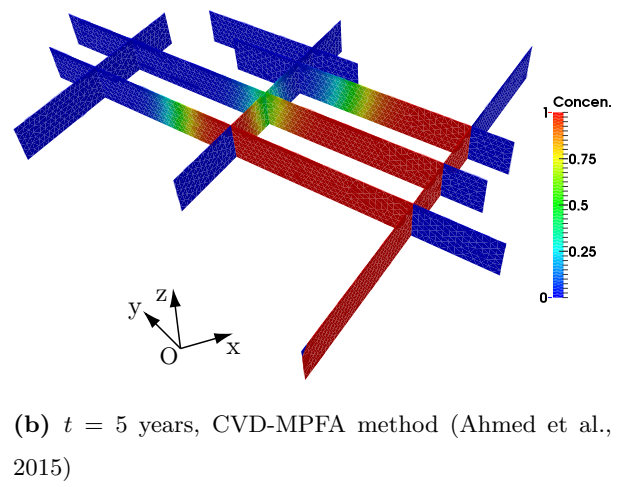
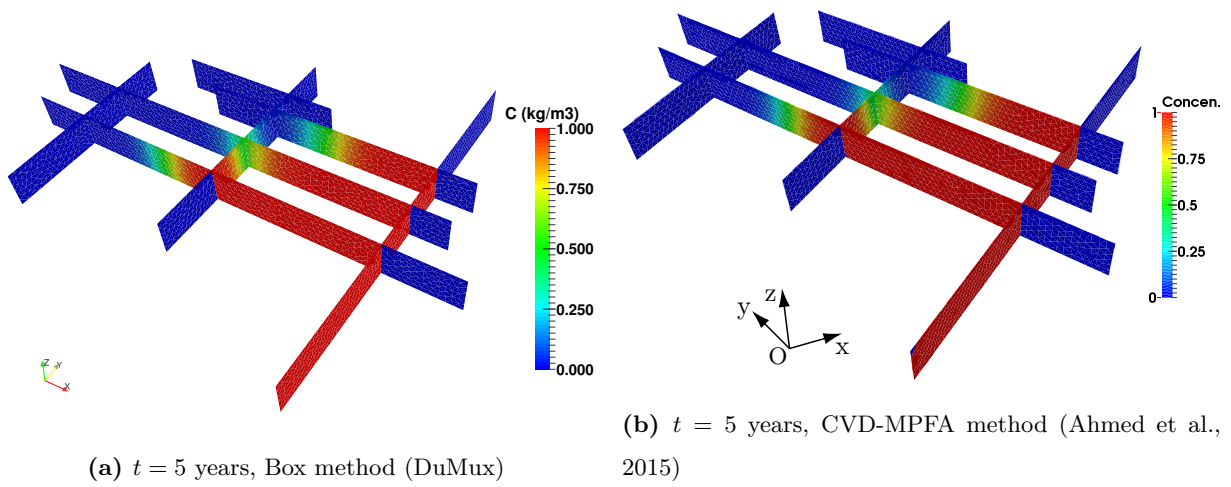


Figure 12: Concentration plots for the 7-fracture DFN.

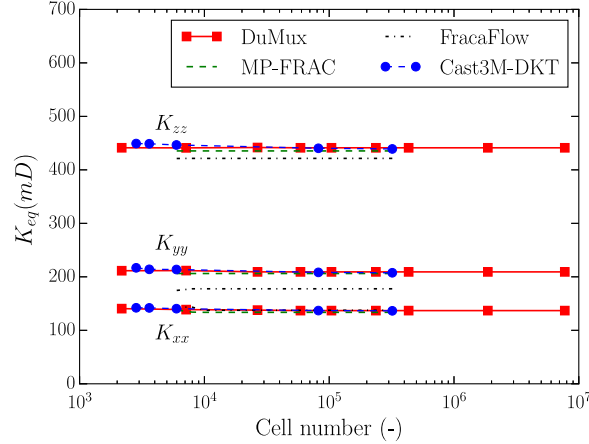


Figure 13: Mesh validation test of the benchmark 33-fracture DFN: equivalent permeabilities computed from the simulation results of single-phase flow at steady-state.

290 Figure 11 shows the locations of the injector I and that of the two producers P_1 and P_2 . Fluid is injected
 291 through the injector at the rate of $2.739 \times 10^{-3} \text{ m}^3/\text{day}$. The imposed pressure at both producers is set to
 292 10 bar. Both gravity and diffusion effects are neglected. Figure 12a illustrates the result of DuMux for the
 293 tracer concentration $t = 5$ years, which matches perfectly with the reference result shown in Figure 12b. An
 294 excellent agreement between concentration plots at the producers P_1 w.r.t time in Figure 12c also validates
 295 our solutions.

296 4.3. Example 3: 33-fracture benchmark synthetic DFN

297 The third validation is undertaken on the DFN₁ based on previous studies by Fournon et al. (2013, 2016).
 298 Firstly, equivalent permeabilities are computed from the numerical solutions of steady-state single-phase
 299 flow and compared with the published results. Secondly, solute transport is modeled and analyzed from a
 300 convergence point of view.

301 To determine the diagonal entries of the effective permeability tensor K_{ii} , $i \in \{x, y, z\}$, a pressure gradient
 302 ΔP is applied on two corresponding opposite boundaries of the DFN and other boundaries are assumed to
 303 be impermeable. The equivalent permeability of a DFN can be calculated by applying the inverse Darcy's
 304 method when the fluid flow is at steady state (Zimmerman and Bodvarsson, 1996).

$$K_{ii} = \frac{\mu \times Q_{ii}}{A \times \Delta P}, \quad (10)$$

305 where Q_{ii} is the corresponding macroscopic flux and A is the cross-sectional area.

306 Note that the off-diagonal terms of the equivalent permeability tensor, i.e. K_{ij} ($i, j \in \{x, y, z\}, i \neq j$), can
 307 also be computed with a different setup of the boundary conditions. However, the calculation of off-diagonal
 308 equivalent permeability is out-of-scope of this work, we only investigate the principal terms K_{xx}, K_{yy} and

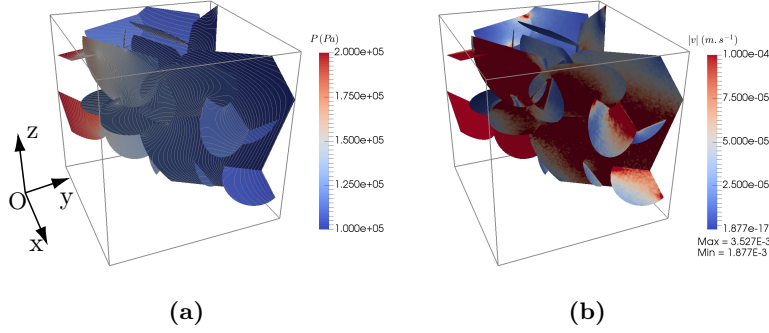


Figure 14: 33-fracture DFN: pressure field and iso-value lines of pressure (a) and the norm of the velocity field (b) from the simulation on a mesh of $h = h_{max} = 0.03$ m.

309 K_{zz} ; the solutions will be used for validation purposes. The DFN is assumed to be homogeneous and isotropic
 310 with the intrinsic permeability is set to 10^4 mD.

311 Figure 13 compares the numerical results of the equivalent permeabilities obtained from simulations with
 312 different codes including DuMux, FracaFlow (Khvoenkova and Delorme, 2011), MP-Frac (De Dreuzy et al.,
 313 2013) and Cast3M (Fournou et al., 2013). One can note that DuMux’s results for the effective permeabilities
 314 along all three principal directions are similar to those obtained by MP-Frac and Cast3M. The results
 315 obtained by FracaFlow are slightly different from the others, but remain of the same order of magnitude.
 316 These discrepancies are caused by the loss of the DFN connectivity in the FracaFlow meshes. Indeed,
 317 Khvoenkova and Delorme (2011) modeled disc-shaped fractures by planar octagons, therefore some DFN
 318 intersections cannot be captured resulting in a consistent underestimation of the equivalent permeabilities
 319 along the y and z directions. On the contrary, it appears that the fracture connectivity in the DFN is
 320 accurately captured by FraC into resulting meshes, that are eligible for flow and transport simulations using
 321 standard simulators.

322 In the experiment of transport through the DFN₁, solute is continuously injected from an inflow boundary
 323 of the DFN. Flow occurs through the DFN along the x -axis by applying a pressure gradient $\Delta P = 10^5$ Pa
 324 along this axis. The dispersion coefficient is isotropic, $D = 10^{-9}$ m².s⁻¹. Simulations are run on different
 325 meshes with the grid size ranging from 1×10^5 elements (coarsest mesh) to 8×10^6 elements (finest mesh). The
 326 characteristic length h varies from $h = h_{max} = 0.03$ m for the coarsest mesh to $h = h_{max}/8 = 3.75 \times 10^{-3}$ m
 327 for the finest mesh,

328 Figure 14a illustrates the pressure field and iso-value lines of the pressure while Figure 14b displays
 329 the norm of flow velocity reconstructed from numerical results using a weighting of the sub control volume
 330 velocities. In Figure 14b, blue colors represent low values (down to 1.877×10^{-17} m.s⁻¹); warmer colors
 331 indicate higher values (up to 3.527×10^{-3} m.s⁻¹). Color scale is set maximum at 1×10^{-4} m.s⁻¹ to distinguish
 332 high- and low-flow regions. We can easily notice from Figure 14 narrowly-spaced pressure iso-value lines for
 333 high-flow regions (for instance, in fractures close to the inlet) and widely-spaced ones for low-flow areas.

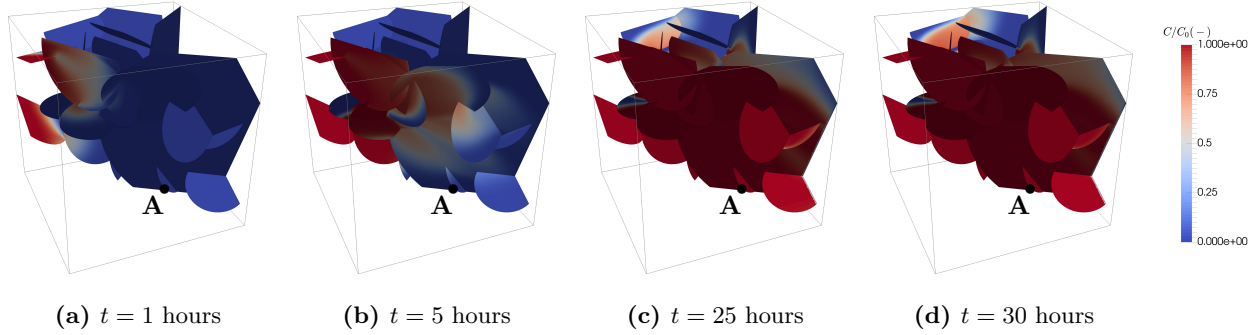


Figure 15: Snapshots of solute concentration distribution over time on the mesh DFN_{16} of mesh size $h = h_{max} = 0.03$ m in Figure 6. Point A illustrates an observation point located at (2.35m, 1.35m, 0m).

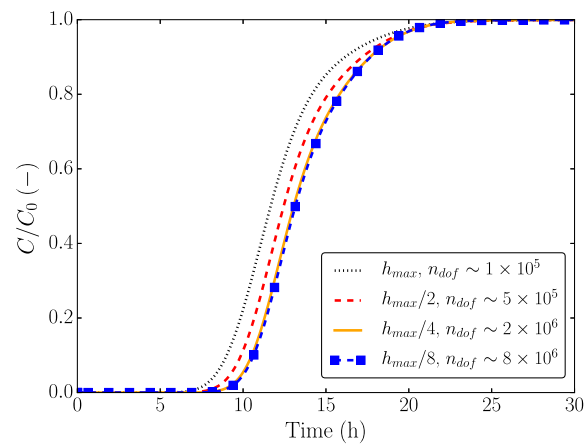


Figure 16: Concentration evolution at the observation point A.

334 Figure 15 shows the tracer concentration distribution of the numerical simulation obtained through
 335 DuMux. It reports the concentration evolution in the DFN at different timescales: after a short time of
 336 injection, $t_1 = 1$ hour (Figure 15a), an intermediate time $t_2 = 5$ hours (Figure 15b) and a relatively long
 337 time $t_3 = 25$ hours (Figure 15c) and $t_4 = 30$ hours (Figure 15d) when the solute has reached the outflow
 338 boundary. We notice that for long times, i.e. after 25 hours, the solute appears nearly in the whole DFN; in
 339 addition, the solute displacement occurs slowly in the DFN, which is expressed through the similar solute
 340 distributions on Figures 15c and 15d. Clearly, this slow motion is the result of both low diffusion effect and
 341 low velocity: the distribution of low concentration areas fits correctly with low-flow regions in Figure 14b.

342 Figure 16 exhibits the concentration evolution at the observation point A of coordinate (2.35m, 1.35m,
 343 0m) obtained from simulations run on 4 grids, the mesh refinement ratio is a factor of 2. Obviously, the
 344 arrival time for coarse meshes is earlier than for fine meshes due to numerical diffusion. The observed curves
 345 obtained from the finest meshes, i.e. the third and fourth grid levels, overlap each other (discrepancy less
 346 than 1%). For instance, the relative concentration at this point at $t = 15$ h for the two coarsest meshes is
 347 about 0.85 and 0.79 respectively, and for both two finest mesh is roughly equal to 0.73. Through this figure,
 348 the convergence of the solution with respect to mesh refinement is also judged.

349 4.4. Example 4: realistic DFN of the Bloemendaal reservoir

350 We study in the last example solute transport within a complex realistic DFN of the Bloemendaal reservoir
 351 with $L_0 = 3$ km. The network contains 3088 fractures and the mesh consists of about 1.1 million grid cells.
 352 As mentioned above, the fracture network is well connected and seems to be homogenizable.

353 Single-phase flow simulations to compute effective permeabilities of the DFN block as described in sub-
 354 section 4.3 are also carried out, giving $K_{xx} = 4.58 \times 10^{-18} \text{ m}^2$ and $K_{yy} = 3.0 \times 10^{-18} \text{ m}^2$. It is worth
 355 noticing that, although there are more y -axis-oriented fractures than x -axis-oriented ones within the DFN,
 356 the effective permeability of DFN along the x -axis is surprisingly about 1.5 times greater than the y -axis
 357 one. This can be explained by the fact that the fracture network is more connected and therefore more
 358 conductive in the x -direction than in the y -direction.

359 Fluid is injected into the domain through an injection well located in the middle of the DFN, the injection
 360 rate is $5 \times 10^{-2} \text{ m}^3/\text{day}$. A Dirichlet condition $P = 10$ bar is applied for all lateral boundaries while a no-flow
 361 Neumann condition is applied for top and bottom boundaries of the domain. As in Example 3, we consider
 362 the case where the dispersion coefficient is isotropic, $D = 10^{-9} \text{ m}^2.\text{s}^{-1}$. Figure 17 shows solute concentration
 363 distribution at $t = 10$ years (Figure 17a), $t = 100$ years (Figure 17b) and $t = 250$ years (Figure 17c).
 364 We note from these figures that there are low-concentration regions which exist locally within the solute
 365 plume. However, disregarding local phenomena, the DFN behaves as a continuous homogeneous medium at
 366 macroscopic scale: the concentration distribution has an elliptical form.

367 In practice, the overall development of a solute plume within a 2D or 3D heterogeneous medium may be
 368 precisely measured through a moment analysis. This approach is an appropriate tool for examining spatial

369 effects of the domain on developing solute plumes, for identifying loss of mass during flow process and for
 370 assessing large-scale dispersive behavior of the flowing domain itself (Freyberg, 1986; Tompson and Gelhar,
 371 1990).

Let us remind that the ijk -th moment of the concentration distribution in space, M_{ijk} is defined as (Aris, 1956)

$$M_{ijk}(t) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \omega C(x, y, z, t) x^i y^j z^k dx dy dz. \quad (11)$$

where ω [-] and C [-] denote the porosity and the relative tracer concentration, respectively. The zeroth-order moment $M_{000}(t)$ is the total mass of the solute in the domain. The first-order moment about the origin, normalized by M_{000} , describes the propagation of the center of mass $O_c(x_c(t), y_c(t), z_c(t))$ of the solute plume:

$$x_c(t) = M_{100}/M_{000}; \quad y_c(t) = M_{010}/M_{000}; \quad z_c(t) = M_{001}/M_{000}. \quad (12)$$

372 The centered second-order tensor defines a spatial covariance tensor reflecting the spreading of mass
 373 about O_c :

$$\bar{\bar{\sigma}} = \begin{bmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{bmatrix} \quad (13)$$

where

$$\begin{aligned} \sigma_{xx} &= \frac{M_{200}}{M_{000}} - x_c^2, & \sigma_{yy} &= \frac{M_{200}}{M_{000}} - y_c^2, & \sigma_{zz} &= \frac{M_{200}}{M_{000}} - z_c^2, \\ \sigma_{xy} &= \sigma_{yx} = \frac{M_{110}}{M_{000}} - x_c y_c, \\ \sigma_{xz} &= \sigma_{zx} = \frac{M_{101}}{M_{000}} - x_c z_c, \\ \sigma_{yz} &= \sigma_{zy} = \frac{M_{011}}{M_{000}} - y_c z_c. \end{aligned}$$

374 Diagonalization of $\bar{\bar{\sigma}}$ provides the orientation of principal axes (x', y', z') as well as the eigenvalues of the
 375 spatial covariance tensor $\sigma_{x'x'}, \sigma_{y'y'}, \sigma_{z'z'}$.

376 In addition, the derivative over time of the covariance is proportional to the dispersion tensor (Aris, 1956;
 377 Freyberg, 1986), one could expect that the square root of the ratio between the eigenvalues of the centered
 378 second-order moments, $\sqrt{\sigma_{x'x'}/\sigma_{y'y'}}$, reflects the anisotropy of the elliptic solute plume for the homogenized
 379 media.

380 Figure 18a reports the variation versus time of the centered second-order moments $\sigma_{xx}, \sigma_{yy}, \sigma_{zz}$ and that
 381 of the eigenvalues of the $\bar{\bar{\sigma}}$ tensor, i.e. $\sigma_{x'x'}, \sigma_{y'y'}, \sigma_{z'z'}$. We note that along the x - and y -axis, the centered
 382 second-order moments and the corresponding eigenvalue match correctly, only a difference between σ_{zz} and
 383 $\sigma_{z'z'}$ is observed. However, since both σ_{zz} and $\sigma_{z'z'}$ are roughly two orders of magnitude less than those
 384 along the x - and y - axis, changing of the z' -axis with respect to the z -axis can also be negligible. This proves

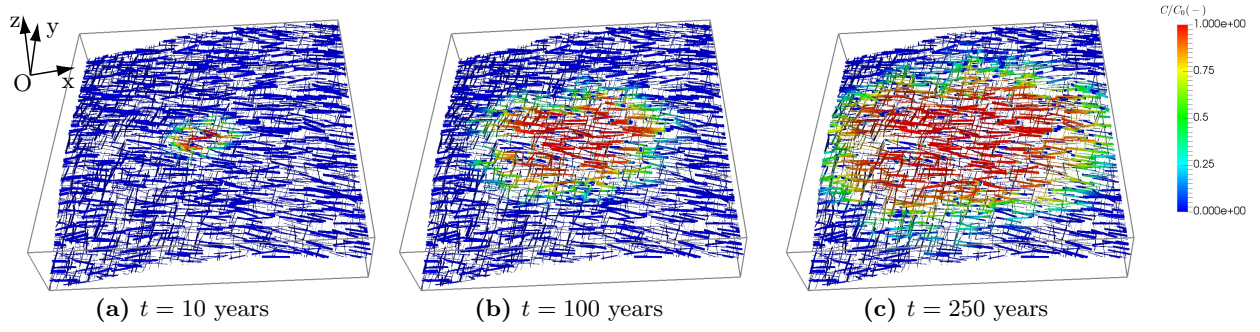


Figure 17: Solute concentration distribution over time on a mesh of $L_0 = 3$ km.

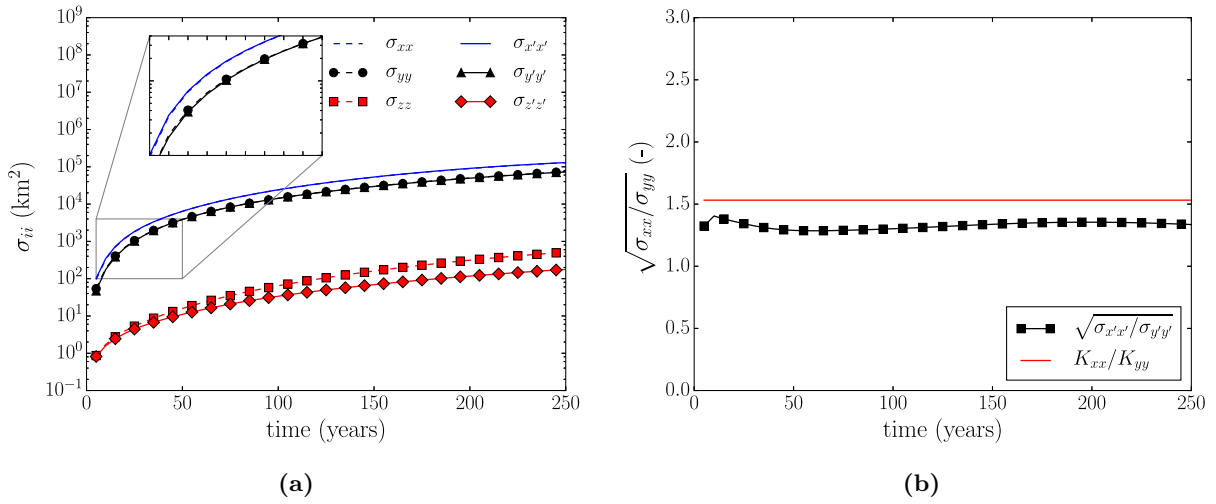


Figure 18: Temporal variation of σ_{ii} ($i \in x, y, z$) (a) and ratio between effective absolute permeabilities K_{xx}/K_{yy} as well as the ratio between the centered second-order moment $\sqrt{\sigma_{x'x'}/\sigma_{y'y'}}$ (b).

385 that the principal axes for the developing direction of the solute plume x', y', z' and the original orientations
 386 x, y, z nearly coincide.

387 Figure 18b illustrates the time-evolution of the $\sqrt{\sigma_{x'x'}/\sigma_{y'y'}}$ ratio. One can notice that $\sqrt{\sigma_{x'x'}/\sigma_{y'y'}}$
 388 is fairly correlated with that of the effective permeabilities K_{xx}/K_{yy} ; a discrepancy exists between them
 389 but it is still acceptable and generally remains stable over time. At early times when the amount of solute
 390 in the domain remains low, $\sqrt{\sigma_{x'x'}/\sigma_{y'y'}}$ is a little greater than the average value because local fracture
 391 connectivity could have significant effects on the ensemble solute distribution. After 50 years, local effects
 392 vanish and the curve becomes relatively stable until 100 years. However, $\sqrt{\sigma_{x'x'}/\sigma_{y'y'}}$ increases slightly
 393 again after 150 years because the solute has already reached lateral boundaries of the DFN.

394 5. Summary and discussion

395 The purpose of this work is to obtain high-accuracy simulations of solute transport within large, three-
396 dimensional Discrete Fracture Networks (DFNs). A workflow is described, including both the mesh genera-
397 tion for DFNs using the conforming mesh method FraC and the simulation framework using the DuMux code.
398 The meshing approach FraC, initially developed by Fournio et al. (2016), relies on the idea of decomposing
399 fractures along extended intersection segments between fractures to obtain a set of interconnected closedW
400 contours, that will then be discretized with the same point density on shared segments between them to
401 ensure the conformity of the final mesh. Conforming meshes were then used for transport simulations with
402 DuMux using a vertex-centered discretization method, or box method. A number of tests were conducted
403 for both validation and demonstration purposes. Validation tests gave satisfactory results: (i) numerical
404 solutions of solute transport on a DFN of single inclined fracture are in agreement with analytical solutions
405 by Ogata and Banks (1961), an a-posteriori convergence analysis showed a convergence rate of $O(h)$ for
406 concentration, where h is the mesh size; (ii) results on 7-fracture DFN obtained by DuMux using the box
407 method match perfectly with those obtained by the cell-centred control-volume distributed multi-point flux
408 approximation (CVD-MPFA) method (Ahmed et al., 2015); and (iii) simulations on a benchmark 33-fracture
409 DFN showed convergence of solution with increasing mesh refinement. Finally, we considered development
410 of solute plume injected into a DFN produced from the Bloemendaal reservoir data that consists of thou-
411 sands of fractures. This test case reveals that our method is able to deal with large-scale DFN containing a
412 moderate fracture number.

413 High-accuracy simulations obtained through this work appear to be very useful for validation of earlier
414 theoretical studies on simplified models, for instance pipe-networks models (Noetinger and Jarrige, 2012;
415 Noetinger, 2015), as well as for benchmarking purposes to test the reliability and performance of commercial
416 or academic simulators. These results also motivate many directions for further works, both for the mesh
417 generation and at the numerical stage. Objectively speaking, numerical simulations on large grids using
418 DuMux could lead to prohibitive CPU times. In order to overcome this issue, several measures could be
419 examined, either adopting the adaptive mesh refinement (AMR) approach (Sander et al., 2015) or distributing
420 the workload on different resources by using parallel computing.

421 It has also been shown that one can only run massively parallel simulations in DuMux if the DUNE
422 grid manager allows it. Nevertheless, to the best of the authors' knowledge, DUNE::FoamGrid is not yet
423 parallelizable. On the contrary, the AMR approach is supported by DUNE::FoamGrid, i.e. simulations can
424 be run on time-evolving meshes with local mesh refinement/coarsening inside DuMux. On the other hand,
425 the AMR approach can be included into FraC frameworks itself without major difficulties. In principle, only
426 vicinity areas of intersections should be refined and a coarse meshing is applied for the remaining. This work
427 can easily be carried out within LaGriT as in the dfnWorks framework (Hyman et al., 2015).

428 Furthermore, although all DFNs in this paper are assumed to be homogeneous for simplicity, the frame-
429 work is, however, able to handle heterogeneity. More precisely, the step S_4 of the FraC approach provides

430 flexibility for both fracture-to-fracture and in-fracture heterogeneity. Heterogeneous parameters such as frac-
431 ture aperture, transmissivity, permeability and porosity are assigned to each mesh element. In the case of
432 fracture-to-fracture heterogeneity, grid cells in a same fracture are assigned a common material index `matID`,
433 the heterogeneous parameters are then distributed according to `matID`. To model inside-fracture heterogene-
434 ity, spatially correlated random fields for fracture aperture are first generated using the R package `gstat`
435 (Pebesma, 2004). The correlation length of random fields λ is proportional to fracture size. Sequential un-
436 conditional Gaussian simulations are carried out to generate random fields for fracture aperture constrained
437 by a simple kriging variogram. The permeability and transmissivity fields are then derived from the aperture
438 distribution using the well-known transmissivity-aperture cubic law (Adler et al., 2012). Heterogeneous data
439 are then directly attached into `*.dgf` grid files and will be read in the DuMux via the DUNE grid interface
440 `DUNE-grid` (Bastian et al., 2008). Preliminary results show that simulations on heterogeneous DFN are in
441 general more time-consuming than on homogeneous ones, hence once again, this highlights the importance
442 of parallel computing.

443 In addition, for the purpose of various applications, more sophisticated problems including, for instance,
444 transient single-phase flow, multi-phase multi-component flow, sorption or reactive transport could also be
445 examined.

446 Finally, another direction to extend our works is to account for the matrix to fracture flow. That may pose
447 challenges for both the mesh generation and simulation procedure. For instance, meshing dense-distributed
448 DFNs with matrix could yield poor quality tetrahedrons that would dramatically degrade numerical per-
449 formances. Furthermore, it requires advanced discretization methods able to deal with the exchange at
450 matrix-fracture interfaces. For that, Vertex Approximate Gradient (VAG) Scheme (Brenner et al., 2015)
451 or cell-centred control-volume distributed multi-point flux approximation (CVD-MPFA) method (Ahmed
452 et al., 2015) could be excellent candidates.

453 **Acknowledgements**

454 The authors would like to thank the Computational Earth Science Group of LANL for providing us the
455 source code of LaGriT and `dfnWorks`.

456 *Counts of words*

457 6560+78+569 (19/18/374/13) Total text+headers+captions

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460 *Counts of characters*

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