Suplementary Information: The hidden structure of hydrodynamic transport in random fracture networks

Marco Dentz[1]†, Jeffrey D. Hyman[2]

[1]Spanish National Research Council (IDAEA-CSIC), Barcelona, Spain.

[2]Computational Earth Science (EES-16), Earth and Environmental Sciences Division, Los Alamos National Laboratory, Los Alamos New Mexico, USA

(Received xx; revised xx; accepted xx)

This supplemental material provides information on the nework generation and meshing, discusses the details of the network considered in the article. Furthermore, it discusses the numerical solution of the flow problem and flow boundary conditions, as well as the numerical solution of the transport problem.

1. Discrete Fracture Network Models: Network Generation and Meshing

We use the discrete fracture network (DFN) methodology to generate fracture networks and numerically resolve flow and transport therein. DFN models are best suited for situations where the fracture network is the primary flow and transport domain and interactions, mass and energy transfer, with the rock matrix can be neglected. In DFN models, individual fractures are explicitly represented as co-dimension one objects, e.g., lines in two dimensions and planes in three dimensions, due to the large contrast in fracture aperture compared to their length. Network generation requires a site characterization to obtain information about the fracture families. However, the amount of data required to constrain generation is limited because measuring subsurface properties, both hydraulic and structural, at the field scale $\mathcal{O}(10^3$ m) is costly and prohibitive (Bonnet et al. 2001; National Research Council 1996; Viswanathan et al. 2022; Zimmerman et al. 1993). In turn, fracture networks are constructed stochastically by sampling distributions, which are parameterized using what limited data is available, for shape, location, and orientation until target parameters, e.g., fracture intensity and density, are obtained. Additional details of DFN models and examples are found in Berrone et al. (2013, 2015); Cacas et al. (1990); Davy et al. (2013, 2010); de Dreuzy et al. (2004); Dershowitz & Fidelibus (1999); de Dreuzy et al. (2012); Erhel et al. (2009); Pichot et al. (2012); Mustapha & Mustapha (2007).

We use the dfnWorks DFN modeling software (Hyman et al. 2015) to perform our simulations. dfnWorks uses the Features Rejection Algorithm for Meshing (FRAM) (Hyman et al. 2014) to create and generate a computational mesh representation of the networks by coupling the two. The former is performed as described above via sampling of appropriate probability distributions, To perform the latter, FRAM uses the near Maximal Algorithm for Poission-disk sampling (nMAPS) (Krotz et al. 2022) to create a variable resolution conforming Delaunay triangular mesh representation of the network. The mesh is refined near intersections to help resolve

† Email address for correspondence: marco.dentz@csic.es

the highest gradients in the physics simulations, which typically occur in proximity to those regions. Upon the fracture planes, the mesh is a two-dimensional manifold, but at intersections, the mesh is three-dimensional. This multi-dimensional mesh allows for straightforward integration of numerical discretizations of governing partial diferential equations without the use of coupling schemes such as Lagrange multipliers or mortar methods. DFNWORKS has been used to explore fundamental aspects of geophysical flows and transport in fractured media (Hyman 2020; Hyman et al. 2019a,b; Kang et al. 2020; Makedonska et al. 2016; Sherman et al. 2020) as well as practical applications including hydraulic fracturing operations (Hyman et al. 2018; Karra et al. 2015; Lovell et al. 2018), inversion of micro-seismicity data for characterization of fracture properties (Mudunuru et al. 2017), the long term storage of spent civilian nuclear fuel (Hadgu et al. 2017), and geo-sequestration of carbon dioxide into depleted reservoirs Hyman et al. (2020).

2. Network Details

We consider a generic network composed of uniformly-sized square fractures with edge length of 2 meters. We consider a cuboid domain of dimensions 100 m × 10 m × 10 m. During the generation stage of the network, the domain expanded one meters in every direction to mitigate low density issues that can arise near the boundaries. Fractures are placed into the domain using a Poisson process, where the centers $\mathbf{c}$ are sampled from a three-dimensional uniform distribution,

$$\mathbf{c} \sim U[-1, 101] \times U[-1, 11] \times U[-1, 11] \ . \tag{2.1}$$

The resulting fracture centers are thus uniformly distributed throughout the domain. After generation is complete, the network is reduced back to the requested domain size,

$$\Omega = [0, 100] \times [0, 10] \times [0, 10] \ , \tag{2.2}$$

where all fracture portions within the domain are retained.

The fracture orientations are sampled from the three-dimensional Fisher distribution,

$$\mathbf{n}(\mathbf{x}; \boldsymbol{\mu}, \kappa) = \frac{\kappa \exp(\kappa \boldsymbol{\mu}^T \mathbf{x})}{4\pi \sinh(\kappa)} \ . \tag{2.3}$$

where $\boldsymbol{\mu}$ is the mean direction vector (T denotes transpose) and $\kappa \geqslant 0$ is the concentration parameter that determines the degree of clustering around the mean direction. Values of κ approaching zero result in a uniform distribution of points on the sphere while larger values create points with a small deviation from mean direction. The Fisher distribution is sampled using the algorithm provided by Wood (1994). We select a mean orientation of $\boldsymbol{\mu} = (0, 0, 1)$ and κ value of 0.1, which produces fractures orientations that are uniformly randomly distributed on the unit sphere and mimic disorderd media (Hyman & Jiménez-Martínez 2017).

The hydraulic aperture of each fracture is constant within each fracture and the same for all fractures, 10^{-5} m. thus, the fracture permeability is $8.3 \cdot 10^{-12}$ m^2 and transmissivity of $9.15 \cdot 10^{-10}$ m^2/s, assuming the fluid is water at 20 degrees C. The fractures are meshed using variable resolution mesh with minimum element size of 0.05 m. The primary mesh is made up of 5,808,681 nodes and 11,557,306 triangular elements. The dual Voronoi mesh has 5,808,681 control volumes.

We initially place 12,000 fractures into the domain. We characterize the network fracture intensity, using the definition provided in Dershowitz & Herda (1992)

$$P_{32} = \frac{1}{V} \sum_{f \in \Omega} S_f \, . \tag{2.4}$$

Here V is the domain volume, S_f is the surface area of the fractures, and the summation over all fractures in the domain. Note that P_{32} has dimensions of $[L^{-1}]$, and its reciprocal P_{32} has dimensions of $[L]$ and is a characteristic length scale of the network, representing an equivalent fracture spacing in three-dimensional space Maillot et al. (2016). The initial network has a P_{32} value of 3.68 m^{-1}, and equivalent spacing of 0.27 m. Next, isolated fractures and isolated clusters of fractures, those that do not connect inflow to outflow boundaries, are removed because they do not participate in flow or transport. Detecting clusters that span the domain and isolated clusters is performed using a graph-based method (Hyman et al. 2017). The final network contains 5,660 fractures has a P_{32} value of 3.12 m^{-1}, and equivalent fracture spacing of 0.32 m.

The fracture network is designed to facilitate insight into and study fundamental features of flow and solute transport and provide a predictive modeling framework. It is not meant to be a realization of a particular field site. In order to observe asymptotic behavior of the transport, we require that the domain be sufficiently long relative to the characteristic fracture size. However, due to computational limitations, the domain cannot be as wide as it is long. During a set of preliminary simulations we determined that our setup is sufficient for observing longitudinal dispersion. We readily acknowledge that such a domain would be inappropriate to observe transverse dispersion due to the limited expansion in the lateral directions.

3. Flow Boundary conditions

In this section we present mathematical forms of the boundary conditions applied within the fractures in the network. We consider a fracture network as a tuple of two sets, one made up the fractures and composed of their intersections. Let $\mathcal{F}$ denote a network of n fractures $\mathcal{F} = \{f_i\}_{i=1}^{n}$. The boundary of each fracture is denoted ∂f. Next, let $I = \{l_{i,j}\}$ be a set of pairs associated with the intersection between fractures, that is, $f_i \cap f_j \neq \emptyset \rightarrow l_{i,j}$. The number of intersections depends on the particular shape, orientation, and geometry of the set of fractures in the network.

Neumann no-flow boundary condition are imposed around the perimeter of all fractures so there is no flow into the matrix through those boundaries,

$$\mathbf{Q}(\mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) = 0 \qquad \forall \qquad \mathbf{x} \in \partial f \tag{3.1}$$

where $\mathbf{Q}(\mathbf{x})$ is the volumetric flow rate, $\mathbf{n}$ is the unit normal vector to the fracture boundary (∂f), and $\cdot$ is the inner product operator. A similar boundary conditions is applied so there is no flow normal to the fracture plane into the matrix,

$$\mathbf{Q}(\mathbf{x}) \cdot \mathbf{n_f}(\mathbf{x}) = 0 \qquad \forall \qquad \mathbf{x} \in f \, . \tag{3.2}$$

Here, $\mathbf{n_f}$ indicates the normal vector of the plane in which the fracture lies.

Next, one needs to impose pressure continuity along fracture intersections.

$$P(\mathbf{x})|_{f_i} = P(\mathbf{x})|_{f_j} \qquad \forall \qquad \mathbf{x} \in l_{i,j} \, . \tag{3.3}$$

where $P(\mathbf{x})|_{f_i}$ denotes the pressure at $\mathbf{x}$ on f_i along $l_{i,j}$. Likewise, the flow is divergence free along intersections.

$$\nabla \cdot \mathbf{Q}(\mathbf{x}) = 0 \qquad \forall \qquad \mathbf{x} \in l_{i,j} \, . \tag{3.4}$$

sNote, that the flux need not be continuous across the line of intersection, as is the case if the values of aperture on the two intersecting fractures are different.

Dirichlet pressure conditions or Neumann flow conditions are assigned along the inflow and outflow boundaries. Without loss of generality, we assume to be the inflow and outflow boundaries to be planes on the sides of the domain. Let $\mathbf{x}_0$ denote points on the inflow boundary and $\mathbf{x}_L$ denote points on the outflow boundary. Dirichelet pressure conditions take the form

$$P(\mathbf{x}) = g_{\mathbf{x}_0}(\mathbf{x}) \quad \forall \quad \mathbf{x} \in \mathbf{x}_0 \quad \text{and} \quad P(\mathbf{x}) = g_{\mathbf{x}_L}(\mathbf{x}) \quad \forall \quad \mathbf{x} \in \mathbf{x}_L\,. \tag{3.5}$$

Neumann flow conditions take the form

$$\frac{\partial \mathbf{Q}}{\partial \mathbf{n}}(\mathbf{x}) = g_{\mathbf{x}_0}(\mathbf{x}) \quad \forall \quad \mathbf{x} \in \mathbf{x}_0 \quad \text{and} \quad \frac{\partial \mathbf{Q}}{\partial \mathbf{n}}(\mathbf{x}) = g_{\mathbf{x}_L}(\mathbf{x}) \quad \forall \quad \mathbf{x} \in \mathbf{x}_L \tag{3.6}$$

4. Flow Simulations

Once the network is generated and meshed, the governing equations for flow (2.3) are discretized using a unstructured two-point flux finite volume scheme, which the community standard in in subsurface flow and transport simulators including FEHM (Zyvoloski 2007), TOUGH2 (Pruess et al. 1999), and PFLOTRAN (Lichtner et al. 2015). The mesh used for computation is the dual of the Delaunay triangulation, the Voronoi tessellation. The Voronoi tessellation is optimal for two-point flux finite volume solvers, in a certain sense being k-orthogonal (Eymard et al. 2000). The discrete version of (2.3) along with boundary conditions(3.1)-(3.4) are used to construct a linear system for pressure at every node in the Voronoi tessellation that ensures volume conservation locally and globally on the Voronoi control volumes. This linear system can be solved using either a direct or iterative method, the choice of which depends on the mesh size and available computational memory (Greer et al. 2022). For the large network we will consider here, we use a Krylov solver (Bi-Conguate gradient stabilized with a Bi-Jacobi preconditioner) implemented within PETSc (Balay et al. 2021) and called by the massively parallel flow and reactive code PFLOTRAN.

We consider flow primarily aligned with the x coordinate, the longest dimension of the domain. Specially, apply Dirichlet boundary conditions for pressure to drive flow from the $\mathbf{x}_0 = 0$m face of the domain to the $\mathbf{x}_L = 100$m face,

$$P(\mathbf{x}_0) = 2 \cdot 10^6 \text{ Pa} \quad \text{and} \quad P(\mathbf{x}_L) = 1 \cdot 10^6 \text{ Pa}\,. \tag{4.1}$$

All nodes in the mesh on the inlet and outlet faces are held constant at these values. This set up creates a pressure difference of 1 MPa across the x-direction, i.e., a hydraulic gradient of 1 MPa / 100 m. The particular value of the pressure difference is arbitrary because our governing equations are linear in ∇P. Therefore, the structure of the steady-flow field does not change with different pressure differences, which is our primary interest, only its magnitude, which can be arbitrary rescaled for our purposes. The selected model set up creates a single principal flow direction, from which the flow within fractures can deviate.

We use the general mode in PFLOTRAN to solve the continuity equation for a single phase, fully saturated, isothermal flow. The governing equation for mass conservation is given by

$$\frac{\partial}{\partial t}(\varphi\eta) + \boldsymbol{\nabla} \cdot (\eta \boldsymbol{q}) = Q_w, \tag{4.2}$$

with Darcy flux $\mathbf{q}$ is defined as

$$\boldsymbol{q} = -\frac{k}{\mu}\boldsymbol{\nabla}\left(P - \rho g z\right). \tag{4.3}$$

Here, ϕ denotes porosity [-], η molar water density [kmol m^{-3}], ρ mass water density [kg m^{-3}], $\mathbf{q}$ Darcy flux [m s^{-1}], k intrinsic permeability [m^2], μ viscosity [Pa s], P pressure [Pa], $\mathbf{g}$ gravity [m s^{-2}], and Q_w is source / sink term. Water density and viscosity are computed as a function of temperature and pressure through an equation of state for water. We set parameters so that gravity is not considered and there are no sinks/sources.

So long as the particular theoretical conditions laid out in Zimmerman & Bodvarsson (1996), i.e., isothermal, laminar, steady flow, are satisfied, then (4.2) is equivalent to (2.3) in the 3D-DFN formulation. Recall that the mesh representation of each fracture is two-dimensional, and the geometric dual mesh of this Delaunay triangulation is a Voronoi tessellation, which is the mesh of control volumes used by PFLOTRAN. To account for the hydraulic aperture of each fracture, the Voronoi control volumes are three-dimensional volumes where the vertical extent is the aperture defined on the nodes of the primary mesh.

We enforce the boundary condition (3.2) by only allowing flow through the lateral boundaries of each control volume. The permeability of each control volume is given by the square of the hydraulic aperture at that point, i.e., we apply a local cubic law within each control volume using

$$k = \frac{b^2}{12} \tag{4.4}$$

By integrating across vertical extent of the control volume, which is the hydraulic aperture at that mesh point, we obtain a third value of aperture and arrive at (2.3).

5. Transport Simulations

The numerical solution provides values of pressure P at every node in the Voronoi tessellation and volumetric flow rates $\mathbf{Q}$ across the faces of the Voronoi control volumes. For particle tracking, however, we desire an Eulerian velocity field $\mathbf{u}(\mathbf{x})$ defined in a three-dimensional Cartesian coordinate system. The use of an unstructured mesh makes this more complicated than dividing $\mathbf{Q}$ by A and ϕ as $\mathbf{Q}$ does not align with the desired Cartesian coordinate system. To this end, we apply the method outlined in Makedonska et al. (2015) and Painter et al. (2012) that uses a least squares method based on the control volume geometry and volumetric flow rates to reconstruct $\mathbf{u}(\mathbf{x})$ at all nodes in the primary mesh. Once $\mathbf{u}(\mathbf{x})$ is obtained, the kinematic equation (2.6) is numerically integrated using an adaptive (spatial and temporal) first-order predictor corrector ordinary differential equation integration method; forward Euler prediction with a backward Euler correction. Bariocentric interpolation is used to obtain the velocity at any point in the domain. Particle behavior within fracture intersections is modeled using a complete mixing assumption where the probability to exit onto a fracture is proportional to the there-into outgoing volumetric flow rate (Berkowitz et al. 1994; Stockman et al. 1997; Park et al. 2001, 2003; Kang et al. 2015; Sherman et al. 2018). Special care is taken during the reconstruction step at intersections to provide vectors from and onto the corresponding fractures. This stochastic method at intersections leads to dispersion of particles with the same initial position, which would otherwise follow the same deterministic pathline through the network. Specifically, we use the numerical method described in Sherman et al. (2018).

We record the travel time, velocity, and position of particles along each pathline.

The adaptive space and time integration results in non-isochronic and non-equidistant samples along the pathline and across the ensemble of particles. To obtain isochronic or equidistant observations, we use linear interpolation to place all particle pathlines onto the same space/time mesh. Additional details about the numerical methods used in the particle tracking are found in (Makedonska et al. 2015; Painter et al. 2012).

REFERENCES

Balay, Satish, Abhyankar, Shrirang, Adams, Mark F., Benson, Steven, Brown, Jed, Brune, Peter, Buschelman, Kris, Constantinescu, Emil, Dalcin, Lisandro, Dener, Alp, Eijkhout, Victor, Gropp, William D., Hapla, Václav, Isaac, Tobin, Jolivet, Pierre, Karpeev, Dmitry, Kaushik, Dinesh, Knepley, Matthew G., Kong, Fande, Kruger, Scott, May, Dave A., McInnes, Lois Curfman, Mills, Richard Tran, Mitchell, Lawrence, Munson, Todd, Roman, Jose E., Rupp, Karl, Sanan, Patrick, Sarich, Jason, Smith, Barry F., Zampini, Stefano, Zhang, Hong, Zhang, Hong & Zhang, Junchao 2021 PETSc/TAO users manual. Tech. Rep. ANL-21/39 - Revision 3.16. Argonne National Laboratory.

Berkowitz, B., Naumann, C. & Smith, L. 1994 Mass transfer at fracture intersections: An evaluation of mixing models. *Water Resour. Res.* **30** (6), 1765–1773.

Berrone, Stefano, Pieraccini, Sandra & Scialo, Stefano 2013 A pde-constrained optimization formulation for discrete fracture network flows. *SIAM J. Sci. Comput.* **35** (2), B487–B510.

Berrone, Stefano, Pieraccini, Sandra, Scialò, Stefano & Vicini, Fabio 2015 A parallel solver for large scale dfn flow simulations. *SIAM J. Sci. Comput.* **37** (3), C285–C306.

Bonnet, Eric, Bour, Olivier, Odling, Noelle E, Davy, Philippe, Main, Ian, Cowie, Patience & Berkowitz, Brian 2001 Scaling of fracture systems in geological media. *Rev. Geophys.* **39** (3), 347–383.

Cacas, M. C., Ledoux, E., De Marsily, G., Barbreau, A., Calmels, P., Gaillard, B. & Margritta, R. 1990 Modeling fracture flow with a stochastic discrete fracture network: Calibration and validation: 2. The transport model. *Water Resour. Res.* **26** (3), 491–500.

Davy, Philippe, Le Goc, Romain & Darcel, Caroline 2013 A model of fracture nucleation, growth and arrest, and consequences for fracture density and scaling. *J. Geophys. Res.-Sol. Ea.* **118** (4), 1393–1407.

Davy, P., Le Goc, R., Darcel, C., Bour, O., de Dreuzy, J. R. & Munier, R. 2010 A likely universal model of fracture scaling and its consequence for crustal hydromechanics. *Journal of Geophysical Research: Solid Earth* **115** (B10).

Dershowitz, WS & Fidelibus, C 1999 Derivation of equivalent pipe network analogues for three-dimensional discrete fracture networks by the boundary element method. *Water Rescour. Res.* **35** (9), 2685–2691.

Dershowitz, William S & Herda, Hans H 1992 Interpretation of fracture spacing and intensity. In The 33th US Symposium on Rock Mechanics (USRMS). American Rock Mechanics Association.

de Dreuzy, J-R, Darcel, C, Davy, P & Bour, O 2004 Influence of spatial correlation of fracture centers on the permeability of two-dimensional fracture networks following a power law length distribution. *Water Resour. Res.* **40** (1).

de Dreuzy, J.-R., Méheust, Y. & Pichot, G. 2012 Influence of fracture scale heterogeneity on the flow properties of three-dimensional discrete fracture networks. *J. Geophys. Res.-Sol. Ea.* **117** (B11).

Erhel, J, de Dreuzy, J-R & Poirriez, B 2009 Flow simulation in three-dimensional discrete fracture networks. *SIAM J. Sci. Comput.* **31** (4), 2688–2705.

Eymard, Robert, Gallouët, Thierry & Herbin, Raphaèle 2000 Finite volume methods. *Handbook of numerical analysis* **7**, 713–1018.

Greer, SY, Hyman, JD & O'Malley, Daniel 2022 A comparison of linear solvers for resolving flow in three-dimensional discrete fracture networks. *Water Resources Research* **58** (4), e2021WR031188.

Hadgu, Teklu, Karra, Satish, Kalinina, Elena, Makedonska, Nataliia, Hyman, Jeffrey D., Klise, Katherine, Viswanathan, Hari S. & Wang, Yifeng 2017 A comparative study of discrete fracture network and equivalent continuum models for simulating flow and transport in the far field of a hypothetical nuclear waste repository in crystalline host rock. *Journal of Hydrology* **553**, 59 – 70.

Hyman, J. D., , Karra, Satish, Carey, J. William, Gable, Carl W., Viswanathan, Hari, Rougier, Esteban & Lei, Zhou 2018 Discontinuities in effective permeability due to fracture percolation. *Mech. Mater.* **119**, 25 – 33.

Hyman, Jeffrey D 2020 Flow channeling in fracture networks: Characterizing the effect of density on preferential flow path formation. *Water Resources Research* **56** (9), e2020WR027986.

Hyman, J. D., Dentz, M., Hagberg, A. & Kang, P. 2019a Emergence of stable laws for first passage times in three-dimensional random fracture networks. *Phys. Rev. Lett.* **123** (24), 248501.

Hyman, J. D., Gable, C. W., Painter, S. L. & Makedonska, N. 2014 Conforming Delaunay triangulation of stochastically generated three dimensional discrete fracture networks: A feature rejection algorithm for meshing strategy. *SIAM J. Sci. Comput.* **36** (4), A1871–A1894.

Hyman, J. D., Hagberg, Aric, Srinivasan, Gowri, Mohd-Yusof, Jamaludin & Viswanathan, Hari 2017 Predictions of first passage times in sparse discrete fracture networks using graph-based reductions. *Phys. Rev. E* **96** (1), 013304.

Hyman, J. D. & Jiménez-Martínez, J. 2017 Dispersion and mixing in three-dimensional discrete fracture networks: Nonlinear interplay between structural and hydraulic heterogeneity. *Water Rescour. Res.* **54** (5), 3243–3258.

Hyman, J. D., Jimenez-Martinez, Joaquin, Gable, Carl W, Stauffer, Philip H & Pawar, Rajesh J 2020 Characterizing the impact of fractured caprock heterogeneity on supercritical CO_2 injection. *Transp. Porous Media* **131** (3), 935–955.

Hyman, J. D., Karra, Satish, Makedonska, Nataliia, Gable, Carl W, Painter, Scott L & Viswanathan, Hari S 2015 dfnWorks: A discrete fracture network framework for modeling subsurface flow and transport. *Comput. Geosci.* **84**, 10–19.

Hyman, Jeffrey D., Rajaram, Harihar, Srinivasan, Shriram, Makedonska, Nataliia, Karra, Satish, Viswanathan, Hari & Srinivasan, Gowri 2019b Matrix diffusion in fractured media: New insights into power law scaling of breakthrough curves. *Geophys. Res. Lett.* **46** (23), 13785–13795, arXiv: https://agupubs.onlinelibrary.wiley.com/doi/pdf/10.1029/2019GL085454.

Kang, P. K., Dentz, M., Le Borgne, Tanguy & Juanes, Ruben 2015 Anomalous transport on regular fracture networks: Impact of conductivity heterogeneity and mixing at fracture intersections. *Phys. Rev. E* **92** (2), 022148.

Kang, Peter K, Hyman, Jeffrey D, Han, Weon Shik & Dentz, Marco 2020 Anomalous transport in three-dimensional discrete fracture networks: Interplay between aperture heterogeneity and injection modes. *Water Resources Research* **56** (11), e2020WR027378.

Karra, S, Makedonska, N, Viswanathan, HS, Painter, SL & Hyman, JD 2015 Effect of advective flow in fractures and matrix diffusion on natural gas production. *Water Resour. Res.* **51** (10), 8646–8657.

Krotz, Johannes, Sweeney, Matthew R., Gable, Carl W., Hyman, Jeffrey D. & Restrepo, Juan M. 2022 Variable resolution poisson-disk sampling for meshing discrete fracture networks. *Journal of Computational and Applied Mathematics* **407**, 114094.

Lichtner, P.C., Hammond, G.E., Lu, C., Karra, S., Bisht, G., Andre, B., Mills, R.T. & Kumar, J. 2015 PFLOTRAN user manual: A massively parallel reactive flow and transport model for describing surface and subsurface processes. Tech. Rep.. (Report No.: LA-UR-15-20403) Los Alamos National Laboratory.

Lovell, A. E., Srinivasan, S., Karra, S., O'Malley, D., Makedonska, N., . Viswanathan, H. S., Srinivasan, G., Carey, J. W. & Frash, L. P. 2018 Extracting hydrocarbon from shale: An investigation of the factors that influence the decline and the tail of the production curve. *Water Resour. Res.* .

Maillot, Julien, Davy, Philippe, Le Goc, Romain, Darcel, Caroline & De Dreuzy, Jean-Raynald 2016 Connectivity, permeability, and channeling in randomly distributed and kinematically defined discrete fracture network models. *Water Resour. Res.* **52** (11), 8526–8545.

Makedonska, N., Hyman, J. D. D, Karra, S., Painter, S. L, Gable, C. W. W &

Viswanathan, H. S 2016 Evaluating the effect of internal aperture variability on transport in kilometer scale discrete fracture networks. *Adv. Water Resour.* **94**, 486–497.

Makedonska, Nataliia, Painter, Scott L, Bui, Quan M, Gable, Carl W & Karra, Satish 2015 Particle tracking approach for transport in three-dimensional discrete fracture networks. *Computat. Geosci.* pp. 1–15.

Mudunuru, M. K., Karra, S., Makedonska, N. & Chen, T. 2017 Sequential geophysical and flow inversion to characterize fracture networks in subsurface systems. *Stat. Anal. Data. Min.* **10** (5), 326–342.

Mustapha, H. & Mustapha, K. 2007 A new approach to simulating flow in discrete fracture networks with an optimized mesh. *SIAM J. Sci. Comput.* **29**, 1439.

National Research Council 1996 Rock fractures and fluid flow: contemporary understanding and applications. National Academy Press.

Painter, S. L., Gable, C. W. & Kelkar, S 2012 Pathline tracing on fully unstructured control-volume grids. *Computat. Geosci.* **16** (4), 1125–1134.

Park, Young-Jin, Lee, Kang-Kun, Kosakowski, Georg & Berkowitz, Brian 2003 Transport behavior in three-dimensional fracture intersections. *Water Resour. Res.* **39** (8), arXiv: https://agupubs.onlinelibrary.wiley.com/doi/pdf/10.1029/2002WR001801.

Park, Y. J., Lee, K. K. & Berkowitz, B. 2001 Effects of junction transfer characteristics on transport in fracture networks. *Water Resour. Res.* **37** (4), 909–923.

Pichot, G, Erhel, J & de Dreuzy, J-R 2012 A generalized mixed hybrid mortar method for solving flow in stochastic discrete fracture networks. *SIAM J. Sci. Comput.* **34** (1), B86–B105.

Pruess, Karsten, Oldenburg, Curtis M & Moridis, GJ 1999 Tough2 user's guide version 2 .

Sherman, T., Hyman, J. D., Bolster, D., Makedonska, N. & Srinivasan, G. 2018 Characterizing the impact of particle behavior at fracture intersections in three-dimensional discrete fracture networks. *Phys. Rev. E* .

Sherman, T., Hyman, J. D., Dentz, M. & Bolster, D. 2020 Characterizing the influence of fracture density on network scale transport. *J. Geophys. Res. Sol. Ea.* **125** (1), e2019JB018547, e2019JB018547 10.1029/2019JB018547, arXiv: https://agupubs.onlinelibrary.wiley.com/doi/pdf/10.1029/2019JB018547.

Stockman, Harlan W, Li, Chunhong & Wilson, John L 1997 A lattice-gas and lattice boltzmann study of mixing at continuous fracture junctions: Importance of boundary conditions. *Geophys. Res. Lett.* **24** (12), 1515–1518.

Viswanathan, H. S., Ajo-Franklin, J., Birkholzer, J. T., Carey, J. W., Guglielmi, Y., Hyman, J. D., Karra, S., Pyrak-Nolte, L. J., Rajaram, H., Srinivasan, G. & Tartakovsky, D. M. 2022 From fluid flow to coupled processes in fractured rock: Recent advances and new frontiers. *Reviews of Geophysics* **60** (1), e2021RG000744, e2021RG000744 2021RG000744, arXiv: https://agupubs.onlinelibrary.wiley.com/doi/pdf/10.1029/2021RG000744.

Wood, Andrew TA 1994 Simulation of the von Mises Fisher distribution. *Commun. Stat. Simulat.* **23** (1), 157–164.

Zimmerman, Robert W & Bodvarsson, Gudmundur S 1996 Hydraulic conductivity of rock fractures. *Transport Porous Med.* **23** (1), 1–30.

Zimmerman, Robert W, Chen, Gang, Hadgu, Teklu & Bodvarsson, Gudmundur S 1993 A numerical dual-porosity model with semianalytical treatment of fracture/matrix flow. *Water resources research* **29** (7), 2127–2137.

Zyvoloski, G 2007 FEHM: A control volume finite element code for simulating subsurface multi-phase multi-fluid heat and mass transfer. *Los Alamos Unclassified Report LA-UR-07-3359* .