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UpsFrac v1.0: An open-source software for integrating modelling and upscaling permeability for fractured porous rocks

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Abstract. Efficient and accurate simulating fluid flow and heat transport underground plays an important role in groundwater migration and geothermal resource prediction, etc. Rock fractures are complex in geological settings, they exhibit multiple scale properties and the fracture pattern is varied for different geological conditions. Modeling and upscaling permeability for fractured porous rocks are both important and sophisticated approaches in the numerical simulation. Nevertheless, there is often a lack of efficient and flexible methods to connect these two processes. In this study, a integrated methodology combining modeling and upscaling permeability for fractured porous rocks in proposed and an open-source software, UpsFrac, is developed to consider complex fracture geometries in discrete fracture models (DFM) that are created determinedly and stochastically. The software can characterize complexity of fractured porous rocks such as power law (fractal) length distribution, correlations between fracture length and aperture, and the effect of rock matrix properties. The state-of-the-art upscaling method, the multiple boundary method (MFU), is applied to calculate equivalent fracture permeability, which links the fine-scale discrete fracture model to the coarse-scale equivalent fracture model. The code is in Matlab and is based on fracture modelling code ADFNE and reservoir simulation code MRST, which can easily run DFM ensembles for uncertainty analysis. The code is available in open repositories to encourage modeling and upscaling of complex fractured porous rocks, allowing users to develop their own routines within the current framework and to benefit a broader community.

1 Introduction

Fractures exist widely in geological settings and are caused mainly by the alteration of geomechanical stress, chemical erosion, and thermal stress (Gu et al., 2020; Gudmundsson, 2011; McDermott and Kolditz, 2006; Molnar et al., 2007; Zoback et al., 2003). These fractures can significantly influence the movement of fluids through rock formations, affecting groundwater flow, contaminant transport, and the overall stability of engineering structures (Cook et al., 2005; Marinos and Carter, 2018; Myers, 2012; Odling and Roden, 1997). In geothermal or petroleum reservoirs, fractures enhance the permeability and porosity, efficiently extracting heat and hydrocarbons (Ghassemi, 2012; Gong et al.,

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2021). Understanding the characteristics and behaviours of fractures is essential for reducing environmental risk, optimizing energy production, and implementing proper management strategies.

Quantitative analysis of reservoirs is essential for predicting sustainable production in geothermal or hydrocarbon systems, which mainly involves data collection, fractured porous rock modelling, upscaling, numerical simulation, and history matching (Andrews et al., 2019; HosseiniMehr et al., 2022; Liu and Reynolds, n.d.; Mejia et al., 2021; Neuman, 2005; Viswanathan et al., 2022). Discrete fractures occur at multiple scales, as illustrated in Fig. 1. Characterizing fractured porous media mainly involves gathering geological, hydrological, and geophysical data to obtain fracture and matrix properties within the reservoir, e.g., fracture orientation, length, density, and connectivity. Once the conceptual model of the fractured porous rock is built based on characterization, there are two primary numerical simulation approaches used to represent these fractures (Berre et al., 2018): the Discrete Fracture Model (DFM) or Discrete Fracture Network (DFN) and the Equivalent Fracture Model (EFM). The Discrete Fracture Model (DFM) approach explicitly represents each fracture within the reservoir, capturing the complexities of fluid flow and its coupled process. The Equivalent Fracture Model (EFM) simplifies the representation by averaging the effects of fractures, making it computationally more efficient while still providing valuable insights. Upscaling techniques are required to calculate equivalent properties and construct a high-efficiency equivalent fracture model (EFM) based on the discrete fracture model (DFM). Furthermore, Accurate upscaling is particularly important for studying the heterogeneity and anisotropy of the reservoir and the existence of representative elementary volume (Wang et al., 2023), allowing for a better understanding of how these factors influence geothermal production (Gottron and Henk, 2021; Rajeh et al., 2019; Renard and Ababou, 2022). Modelling and upscaling discrete fracture models are prerequisites for the following numerical simulations and history-matching procedures.

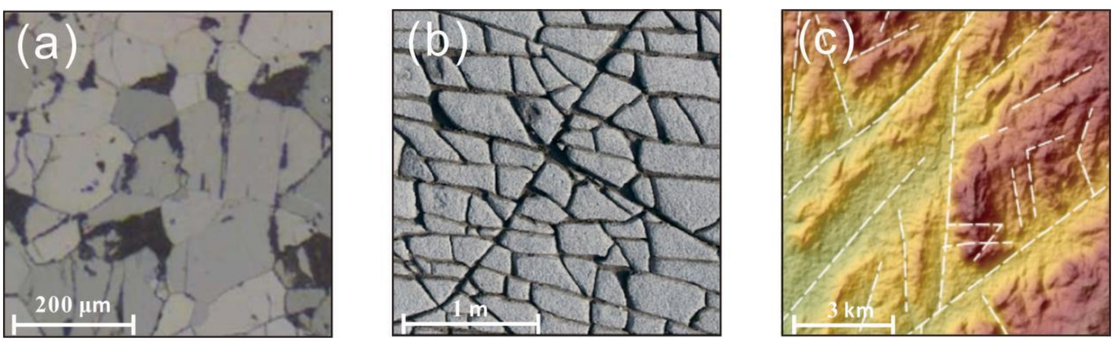

Figure 1: Multiple-scale fractures in geological settings. Adapted from Cheng and Wong (2018), Palamakumbura et al. (2020), and Weismüller et al., (2020).

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Fractures are complex in their geometries and introduce uncertainty in the model, primarily due to limited data availability and the influence of dynamics of rock and fluid underground (MacQuarrie and Mayer, 2005; Srinivasan et al., 2018), which poses significant challenges in accurately characterizing and modelling fractured porous media. Numerous codes have been developed to advance such media's characterization and modelling processes to address these issues. Hardebol and Bertotti (2013) developed DigiFract, a software solution that enables comprehensive fracture data collection from outcrops with greater efficiency than conventional surveying methods, enabling faster collection of larger and more accurate fracture datasets for better characterization of fractured rocks. Healy et al. (2017) developed FracPaQ, an open-source MATLAB™ toolbox designed for quantifying fracture patterns from two-dimensional images in multiple scales, such as thin section micrographs, geological maps, outcrop or satellite images. Alghalandis (2017) developed an open-source software ADFNE for stochastic modelling of discrete fracture networks in two- and three-dimensional applications. ADFNE provides a platform for visualizing and analyzing fracture networks, offering a valuable tool in fractured rock mechanics. Welch et al. (2020) developed DFN Generator v2.0, an innovative tool that simulates natural fracture network evolution based on geomechanical principles rather than stochastic methods, enabling more realistic modeling of fracture networks at kilometer scales. Ovaskainen (2023) developed the Python package fractopo, which provides tools for data validation and analysis of fracture trace observations digitized from base maps like drone images of outcrops or digital elevation models.

More recently, Borghini et al. (2024) introduced the Fracture Analyser, a simple and immediate Python tool, for the 2D analysis of fracture patterns in rock outcrops. The tool quantifies number, length, orientation, position, fracture density, etc., providing an efficient, flexible and accurate tool for the characterization and modelling of natural fractures. There are some open-source codes for modelling flow and coupled processes in fractured porous media, such as OpenGeoSys (Kolditz et al., 2012), PorePy (Keilegavlen et al., 2021), SHEMAT-Suite (Keller et al., 2020). Nevertheless, there is still a gap between linking such fracture geometric properties to the equivalent properties of the equivalent fracture model when doing numerical simulation. To our best knowledge, few codes exist on integrated modelling and upscaling for fractured porous rock.

UpsFrac is an advanced software platform that bridges the traditional gap between modeling and upscaling of fractured porous rocks through innovative integration strategies. It can combine both stochastic and deterministic fracture models, allowing for a comprehensive representation of fracture networks. A distinguishing feature is the ability to generate fractal discrete fractrue models, i.e., power law length distribution (Corral and González, 2019), and establish correlations between aperture and length, which are crucial for understanding fluid flow behaviour in natually fractured systems. UpsFrac employs Two-Point Flux Approximation (TPFA) or Multi-Point Flux Approximation

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(MPFA) schemes for solving flow equations in discrete fracture models (Sandve et al., 2012) and the multiple boundary upscaling method (Chen et al., 2015), providing an accurate and efficient upscaling approach. This method enhances the predictive capabilities of simulations by creating an ensemble of realizations that reflect the uncertainty in the discrete fracture model. As a result, users can estimate reservoir performance while accounting for the complexities of fracture geometries. Furthermore, the open-source code in MATLAB offers significant advantages. It is user-friendly and easily modifiable, allowing researchers to revise the software to specific scenarios or requirements. This flexibility makes UpsFrac a tool for modelling and upscaling applications, enabling users to explore various fracture configurations and their impacts on reservoir behaviour.

2 Software Discription

UpsFrac software has three main components: modelling fractured porous rocks, fractured porous media upscaling and equivalent permeability visualization. For the fractured porous rock modelling part, the Matlab code ADFNE (Fadakar Alghalandis, 2017) is required for the supply basic function to create discrete fracture networks. For the flow-based upscaling procedure, the Matlab code MRST (Lie, 2019) is applied to solve the flow equations in the discrete fracture model. The detailed workflow of UpsFrac is shown in Fig. 2.

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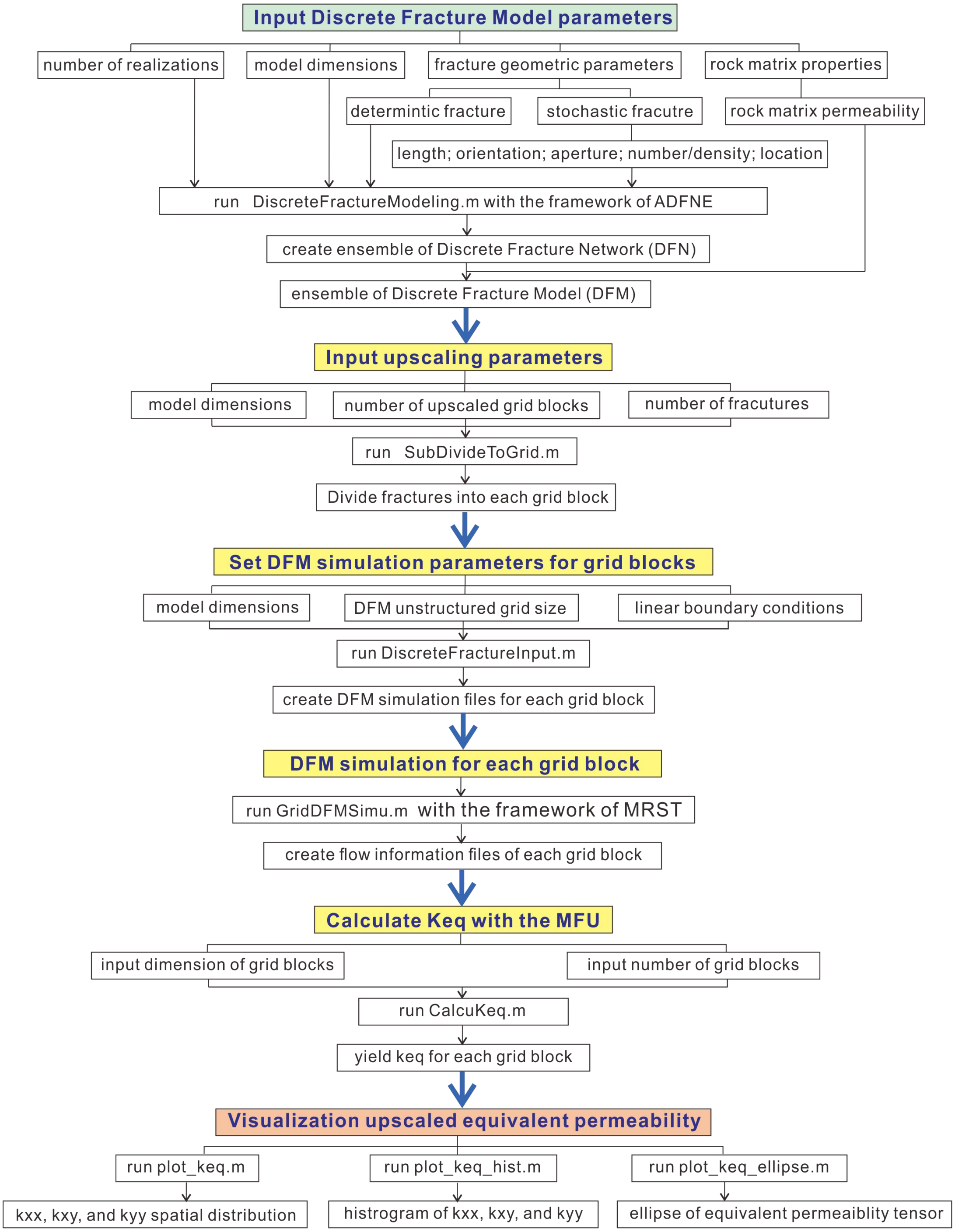

Figure 2: Workflow of the software UpsFrac.

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2.1 Modeling fractal fractured porous rock

The two-dimensional domain should be defined, e.g., as a rectangle by Lx and Ly, for modelling fractured porous rocks. The discrete fracture model can consider the discrete fracture network as well as the rock matrix. Modelling fractures include deterministic and stochastic fractures. After the fracture geometries are defined, the rest of the domain is filled with the rock matrix. The matrix can be characterized by permeability, porosity, etc.

For deterministic fractures, two endpoints, A(x1, y1) and B(x2, y2), and the fracture aperture should defined for each fracture. The deterministic fracture is usually defined for fractures with large scale, e.g., fault or fractures with low uncertainty and is important for conducting flow and heat transport. The deterministic fracture can be stored in the file frac_deterministic.txt. Each line contains geometric data of a fracture.

For stochastic fractures, the discrete fracture network is determined by different geometrical properties(Bonnet et al., 2001) , such as fracture length, aperture, position, and orientation (Xu and Dowd, 2010). The stochastic fracture is mainly based on the software ADFNE. Furthermore, UpsFrac is capable of modelling the truncated power-law length distribution which describe the fractal characteristics of natual fractures. The probability density function for the fracture length l can be written as (Corral and González, 2019; Hyman et al., 2016; Massart et al., 2010):

$$n(l) = \frac{\alpha-1}{l_{min}(1-(\frac{l_{min}}{l_{max}})^{\alpha-1})}(\frac{l_{min}}{l})^{\alpha}, \tag{1}$$

where l_{min} and l_{max} are the lower and upper bound of the fracture length, α, ranging from 1.3 to 3.5, is a power-law exponent influenced by the growth properties of fractures (Bonnet et al., 2001).

Furthermore, the fracture aperture, w, can be correlated to fracture length in UpsFrac by the following power law expression:

$$w = \gamma l^{D}, \tag{2}$$

where γ is the coefficient related to mechanical properties of fractured rocks and D denotes the correlation exponent, which signifies the mechanical interaction among closely positioned fractures. D may vary from 0.5 to 1 resulting from the observations in the field. $D = 0.5$ represent complex open-mode fractures with a constant fracture toughness (Klimczak et al., 2010; Olson, 2003). $D = 1.0$ occurs in faults and shear deformation bands under constant driving stress (Vermilye and Scholz, 1995).

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Users can use the ADFNE framework to create stochastic realizations for fracture orientation, density, and location. Furthermore, users can develop their models to create stochastic fractures. All the fracture geometric parameters are defined in DiscreteFractureModeling.m script. The output file for discrete fracture models is in *.txt format, which is easy to read and can be applied to the following processes.

2.2 Upscaling permeability for fractured porous media

The upscaling procedure mainly involves finding the equivalent properties on coarse-scale grid blocks based on the information from fine-scale discrete fracture models. The first step is to divide the fracture into cartesian grids. The cartesian grid numbers in the x and y direction, nx and ny, should be defined. This step is accomplished in the script SubDivideToGrid.m, where each fracture is looped and clipped into a cartesian grid defined by nx and ny. This step yields an output file with .txt format. Each line represents the clipped fracture in a Cartesian grid, which includes the sequence number of the grid ranging from 1 to nx*ny, two endpoints (Fig. 3), A (x1, y1) and B (x2, y2), and the aperture of the fracture. We should note that the dimension of the Cartesian grid is (Lx/nx)×(Ly/ny); accordingly, the start and end points of the fractures A (x1, y1) and B (x2, y2) are in the range of the cartesian grid dimensions.

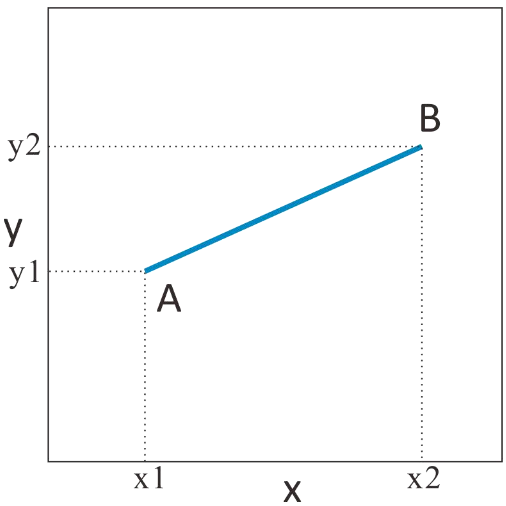

Figure 3: Schematic diagram of a fracture represented by endpoints A and B.

Next, the clipped fractures are combined into a discrete fracture network for each cartesian grid and saved as input files for numerical simulations by the discrete fracture model. The model is based on MRST code and is solved using the Two-point Flux Approximation (TPFA) or Multi-point Flux Approximation (MPFA) scheme (Sandve et al., 2012), which can accurately and robustly model fluid flow in highly heterogeneous media. We should note that each grid block usually has the same grid dimensions and rock matrix properties; only the fracture geometries differ. Therefore, we can slightly change a based template file, InputTemplate.m, regarding fracture geometries for the different cartesian

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grids. We should also note that even though the dimensional and matrix properties for the cartesian grid are the same, when the dimension of the model changes, the grid size of the fracture and rock matrix in the discrete fracture mode should also be adjusted for meshing and modelling the discrete fracture model for the cartesian grid. In this step, the numerical modelling code for each cartesian grid containing fracture is created, and the combined fracture geometries data are stored for the following equivalent permeability calculation.

Then, the numerical simulations for cartesian grids that contain fractures are conducted using the framework of the MRST code. For each grid, two simulations are conducted that the pressure gradient along the x and y-axis. The results used for upscaling are saved, including the flux, the centre of the face, and the index of the grid face (fracture or matrix). If the grid block does not contain fractures, the matrix permeability is defined for the grid block.

Subsequently, the multiple boundary method is applied to calculate the equivalent permeability for each grid block by applying the previous simulation results. The multiple boundary method uses multiple boundary expressions to calculate flux. When the linear boundary conditions are applied along the x-axis, the flow rates along the x- and y-axis, q_x and q_y, are calculated on multiple boundaries:

$$\begin{aligned} q_{\mathrm{x}} &= \int_0^{l_{\mathrm{y}}} v_{\mathrm{r}} \cdot n_{\mathrm{x}} \mathrm{d}y + \int_0^{l_{\mathrm{x}}} v_{\mathrm{u}} \cdot n_{\mathrm{x}} d\mathrm{x} + \int_0^{l_{\mathrm{x}}} v_{\mathrm{l}} \cdot n_{\mathrm{x}} \mathrm{d}x \ , \\ q_{\mathrm{y}} &= \int_0^{l_{\mathrm{x}}} v_{\mathrm{u}} \cdot n_{\mathrm{y}} \mathrm{d}\mathrm{x} + \int_0^{l_{\mathrm{x}}} v_{\mathrm{l}} \cdot n_{\mathrm{y}} d\mathrm{x} + \int_0^{l_{\mathrm{y}}} v_{\mathrm{r}} \cdot n_{\mathrm{y}} \mathrm{d}y \ , \end{aligned} \tag{3}$$

where l_x and l_y are dimensions of the Cartesian grid in the x- and y-directions, n_x and n_y are unit vectors along the x- and y-axes, v_r, v_u, and v_l denotes the Darcy velocities on the right, upper, and lower boundaries.

Lastly, the coarse-scale equivalent permeability can be computed inversely based on the Darcys law using the flux in the fine-scale discrete fracture model. The details of the multiple boundary methods can be found in Chen et al.(2015). In this step, the run code CalcuKeq.m yields an epcomf.txt. Each line in epcomf.txt contains the sequence number of coarse grid blocks, the components of equivalent permeability kxx, kxy, kyx and kyy.

2.3 Equivalent permeability visualization

The upscaled equivalent permeability can be further analyzed and visualized by using FracUpM. The resulting equivalent permeability is a full tensor form and is not inherently symmetric for fractured rocks (Chen et al., 2016; Zijl and Stam, 1992). To simplify, a symmetric permeability can be calculated by averaging the off-diagonal components.

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Using the upscaling results, the permeability distribution of different components, kxx, kxy and kyy, can be plotted using the code plot_keq.m. The spatial heterogeneity and anisotropy of equivalent permeability can be characterized. Furthermore, to analyze the statistical properties of the equivalent permeability, the histogram of equivalent permeability components can be plotted using the codel plot_keq_hist.m. The histogram is important for building a stochastic field of equivalent permeability (Fiori et al., 2015). Lastly, the equivalent permeability tensor of a grid block can be visualized using an ellipse; this can be done using the code plot_keq_ellipse.m, in which the directional properties of equivalent permeability can be presented more understandably.

3 Validation

3.1 Fractrue with power law length distribution

For modelling the fracture length with power law distribution, the cut-off power law is applied to create fracture length. For fractures with length l ranging from l_{min} to l_{max}, the power law distribution can be expressed as in equation (1). The power law distribution for fracture length is created using the rndm_powerlaw function. The values of l_{min}, l_{max}, power-law exponent α and fracture number N should be determined. For instance, when l_{min}=10 m, l_{max}=1000 m, α=2.5, and N=500, the histogram of stochastically generated fracture length is plotted in Fig. 4, which exhibits a long/short tail as alpha is high. When fitting the stochastically generated data with the maximum likelihood estimation method, the fitted α is 2.52, close to the input alpha 2.5. The Kolmogorov-Smirnov statistic is 0.032, indicating that the software UpsFracM generates the data set and agrees with the fitted power-law distribution.

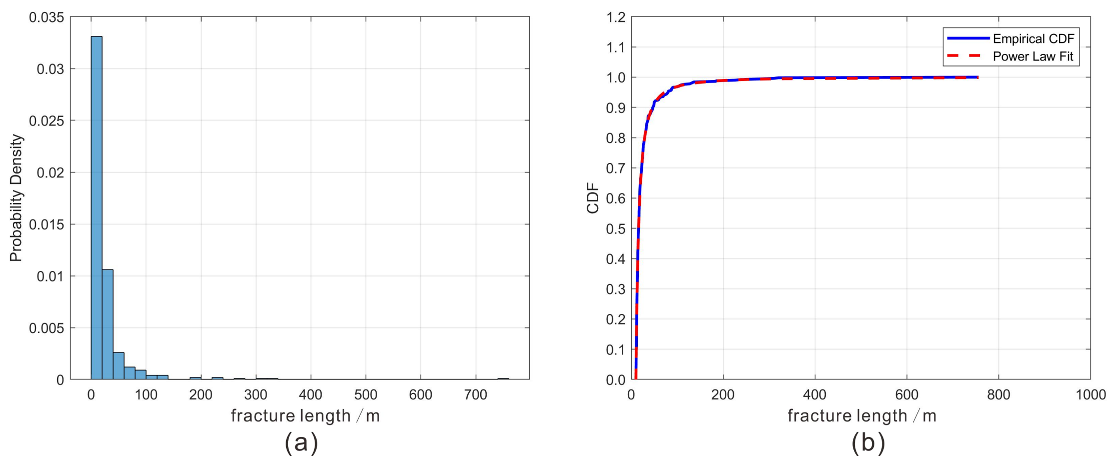

Figure 4: (a) Histogram of power law distribution, (b) Cumulative Distribution Function (CDF) of created data and fitted power law.

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3.2 Equivalent fracture permeability with varied aperture

The UpsFrac software is capable of correlating fracture aperture and fracture length with the power law function, i.e., equation (2) for modeling fractured porous rocks. For testing the accuracy of the upscaling results, the equivalent permeability of fracture with varied aperture is calculated with the UpsFrac. It is compared with the analytical solution (i.e., compute flux analytically) of equivalent permeability. When γ is assumed to be 1.2×10^{-4}, the correlation exponent D ranged from 0 to 1, the equivalent permeability calculated by UpsFrac ranged from 0.7×10-13 m2 to 5.8× 10-13 m2, showing good agreement with the equivalent permeability calculated analytically (Fig. 5). The validation shows UpsFrac can handle complex fractures with varied apertures, and the equivalent permeability can be calculated accurately. Furthermore, other aperture models can also included easily in the framework UpsFrac. Here is the fracture aline with the grid block boundary in the x-axis, for the fracture with a azimuth of fracture boundary, the multple bounday upscaling method implemented in UpsFrac can also yield a perfect agreement with the analytical method (Chen et al., 2015).

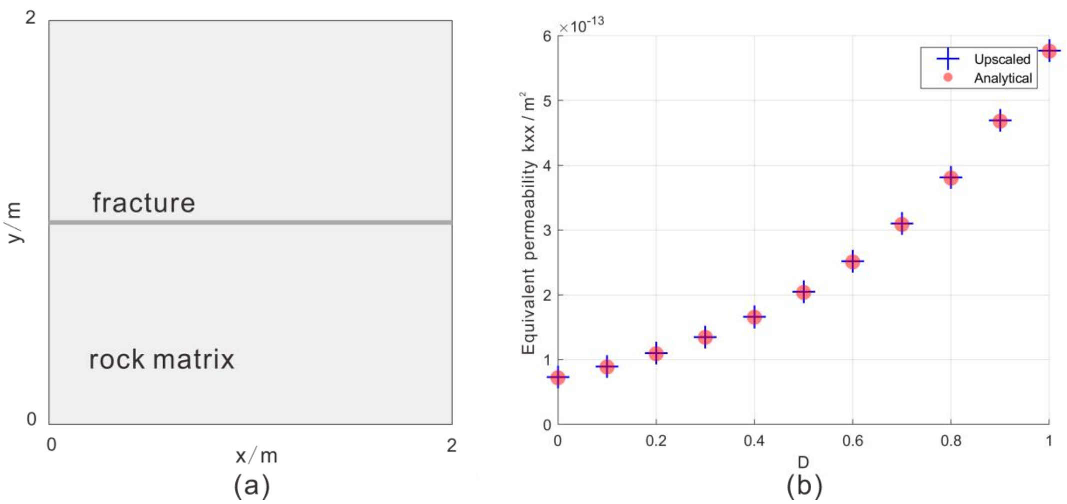

Figure 5: Comparison of upscaled and analytical equivalent permeability for varied aperture models.

4 Sofwtare application

The modelling and upscaling procedure is applied to a real-scale problem by using UpsFrac. Considering the dimension of the model is 1000m × 1000 m. The domain contains both large-scale fractures (faults) and small-scale fractures, referring to the measured data in the field (Massart et al., 2010). The fracture contains both deterministic fractures and stochastically generated fractures. The deterministic fractures include three fractures with an aperture of 0.001 m. The stochastic fracture length follows a power law distribution, with l_{min}=10 m, l_{max}=1000 m, N=200, and α =2.5. Fracture orientation follows Fisher distribution with κ =0, meaning the fracture orientation is randomly

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distributed. Fracture location follows uniform distribution. In this study, the aperture is correlated with fracture length with γ of 2.3×10^{-5} and D of 0.5 according to the field data (Schultz and Soliva, 2012). The above geometric data are input in the script DiscreteFractureModeling.m. The rock matrix permeability is homogeneous and isotropic with 9.87 ×10-16 m2. One realization of the discrete fracture model is shown in Fig. 6.

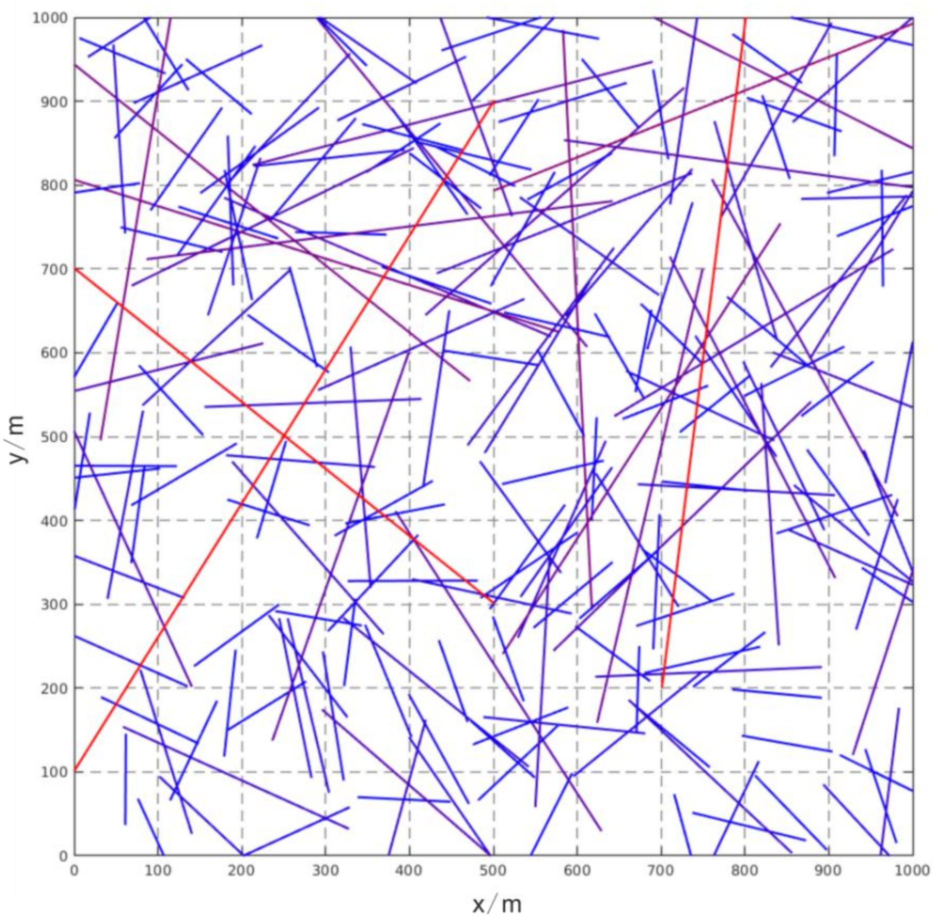

Figure 6: Discrete fracture model generated by UpsFrac. Blue denotes a low aperture, red denotes a high aperture, and the dashed line denotes the grid blocks on a coarse scale.

The grid block size for upscaling is 100 m × 100 m. which is the input parameter in the script SubDivideToGrid.m. Each grid contains 3-9 fractures clipped by the grid boundaries. For the numerical simulation of each grid, the unstructured mesh size for the rock matrix is 5 m, and for fracture, it is 3.3 m. After simulating fluid flow in all grid blocks, the required information for upscaling is calculated. By running the script CalcuKeq.m, the equivalent permeability for each grid block is calculated.

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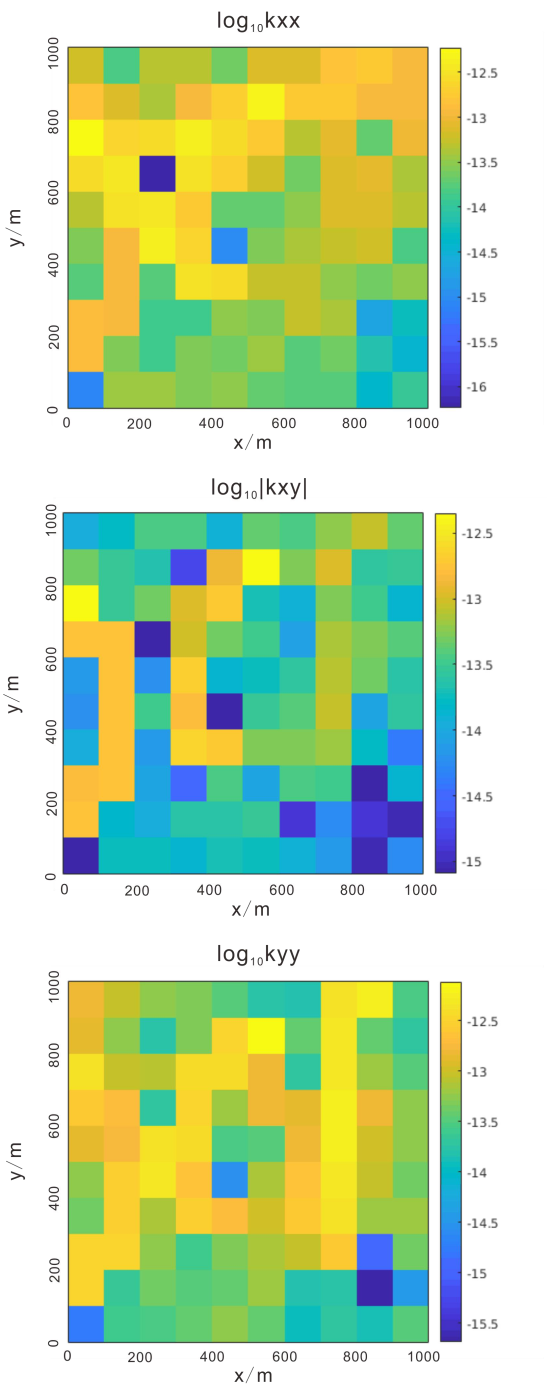

Figure 7: Equivalent permeability distribution of grid blocks on a coarse scale.

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The resulting equivalent permeability is plotted by running the script plot_keq.m based on the calculated equivalent permeability file epcomf.txt and the grid number in the x- and y-axes, nx and ny. The equivalent permeability distribution shows that it is highly correlated with the geometries of fractures (Fig. 7). Different components of equivalent permeability are different, which is influenced by the fracture orientation.

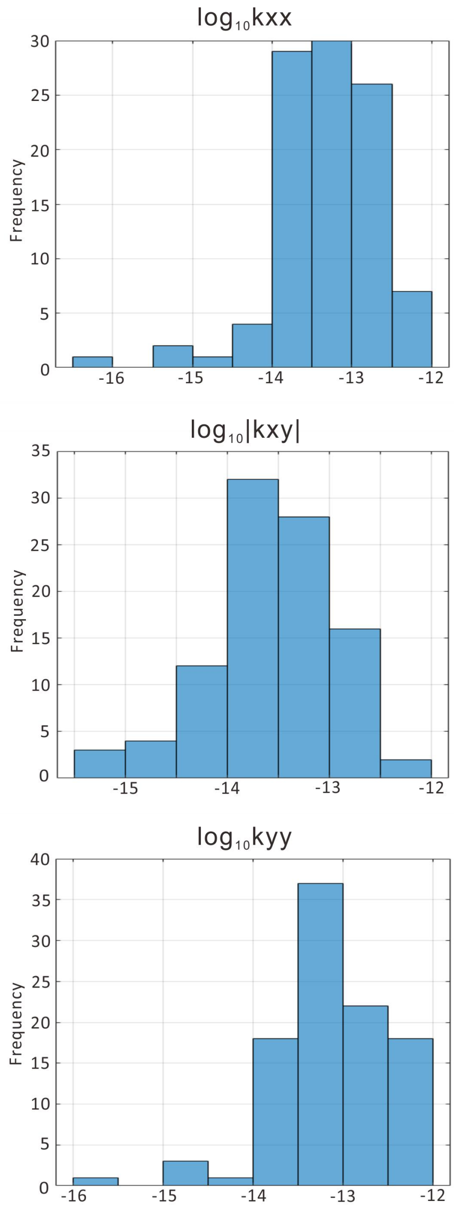

Figure 8: Histograms of upscaled equivalent permeability components.

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The histogram of different components of equivalent permeability is plotted in Fig. 8. It shows that it follows a log-normal distribution for all components k_{xx}, k_{xy}, and k_{yy}. For k_{xy}, it can be positive and negative; we use the absolute value here for plotting. For k_{xx} and k_{xy}, the shapes of histograms are similar. The results indicate that even though the spatial distribution is different, the statistical properties of k_{xx} and k_{xy} are similar. This is mainly due to the that the orientation is randomly distributed, i.e., without a preferable orientation. For k_{xy}, it slightly lower than k_{xx} and k_{xy}; this is consistent that the permeability tensor is positive definite (Lang et al., 2014).

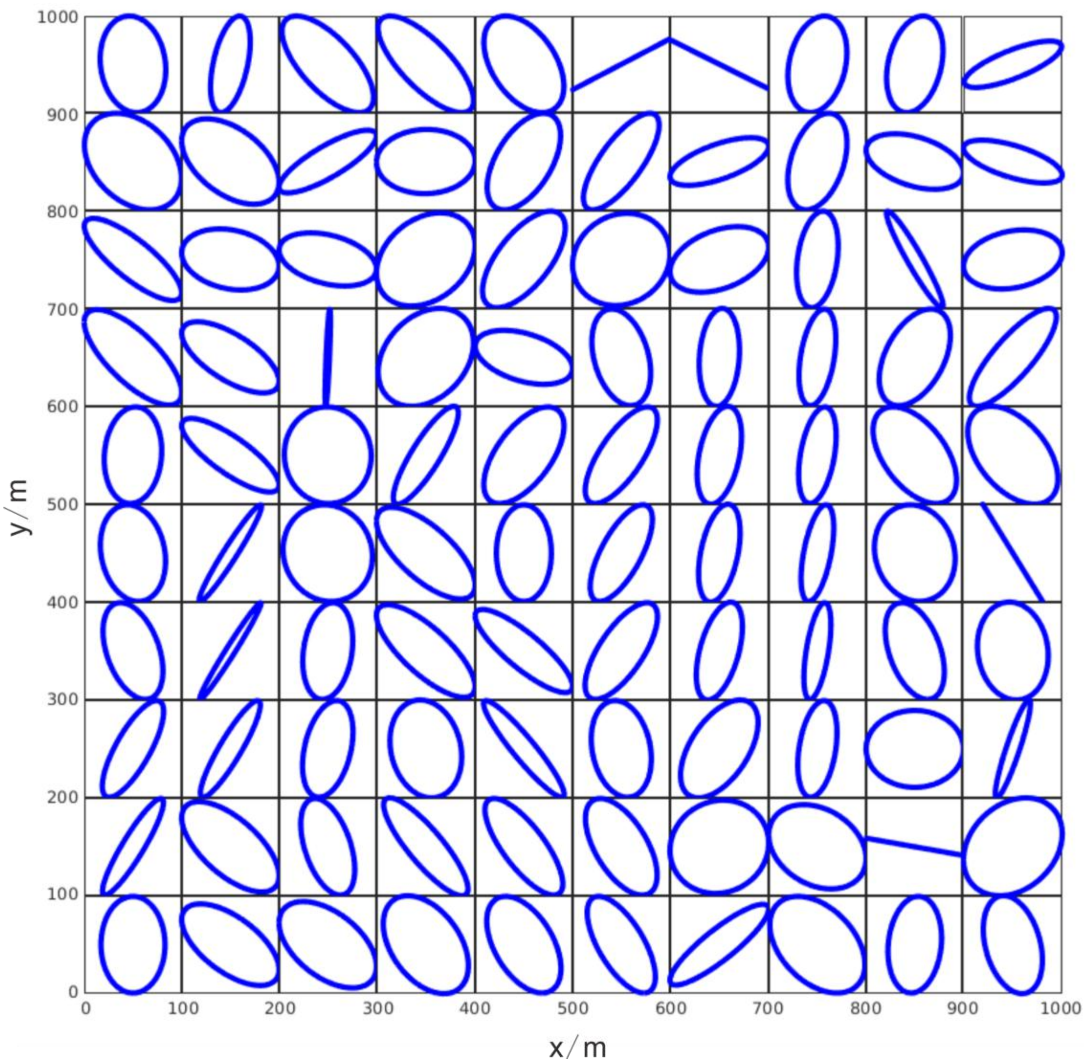

Figure 9: Ellipse of equivalent permeability tensor for the model.

The permeability tensor can be visualized using the ellipse. The permeability ellipse for all grid blocks is plotted in Fig.

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9. It shows that the long axis of an ellipse follows the fracture orientation (Fig. 6), especially for the grid with a few large fractures with high permeability (e.g., the grid block near the lower left corner of the model). The consistent shape of the upscaled permeability tensor ellipse and the geometries of the fracture network indicate the upscaling codeUpsFrac yield reasonable and accurate results. Which can be used for characterizing the permeability of the fractured rock and further as the input of equivalent fracture models.

5 Limitions and future developments

The modelling and upscaling fractured porous media code UpsFrac assumes that the aperture of the fracture is constant for one single fracture, although it can handle different apertures for different fractures. Further improvement could consider the heterogeneity of a single fracture, i.e., the varied aperture due to the fracture surface roughness results in a non-uniform permeability for the single fracture (Li et al., 2022; Xue et al., 2022).

UpsFrac can theoretically run accurately for upscaling permeability. In contrast, numerical stability needs to be considered in the upscaling process, which needs to numerically solve fluid flow equations in a discrete fracture model. Therefore, accurately solving the flow equation in very complex fractured porous needs to adjust some parameters, such as the mesh size of the fracture and rock matrix. To prohibit the unsuccessful simulation and yield an accurate equivalent permeability, the grid blocks with no fractures or numerically solved successfully are documented in .txt files. By checking these simulation information files, the user can adjust the overall template input files for numerical simulation on grid blocks or modify the input files of the individual grid blocks. In the future, machine learning techniques can be used instead of solving flow equations in discrete fracture models (Almajid and Abu-Al-Saud, 2022; X. Yan et al., 2024) to yield efficient results regardless of the adjustment of the grid size of the discrete fracture model.

The UpsFrac applies the Multiple boundary methods for calculation equivalent permeability, which is accurate as a flow-based method; other fast analytical upscaling methods (Ebigbo et al., 2016; Oda, 1985), such as Effective

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Medium Theory (EMT), can also easily be implemented in the framework of UpsFrac for upscaling permeability for fractured porous rocks. The software can be further developed for enhancing a wider and more convenient applications. Key areas for improvement include the user interface, software stability, and compatibility with other reservoir simulation tools. This can be achieved through standardization of data formats and the development of API interfaces, which will facilitate broader adoption in industrial settings (M. Yan et al., 2024).

6 Conclusions

The paper describes a new free and open-source software UpsFrac for modelling and upscaling permeability for two-dimensional fractal fractured porous rocks. The software supplies a methodology for creating multiple-scale fractures with varied apertures, including deterministic and stochastic. The complex relations between fracture length, fracture density, and fracture aperture can be easily implemented in the framework of UpsFrac. The software applied the state-of-the-art upscaling method, the multiple boundary method, which is a flow-based upscaling approach based on the Two-Point Flux Approximation (TPFA) scheme or Multi-Point Flux Approximation (MPFA) and supplies accurate and robust upscaling results.

The software aims to provide a flexible toolbox for creating fractured porous rocks with complex fracture geometries. The discrete fracture models can be upscaled to calculate equivalent permeability. The software is useful for investigating the heterogeneous and anisotropy of equivalent fracture permeably for fractured porous rocks and further as input parameters in the equivalent fracture models. All the code and application scripts are available for download.

Author contribution

TC: Conceptualization, Writing-original draft, Software, Investigation, Formal analysis, Funding acquisition. HS: Writing-review & editing, Methodology, Validation, Visualization. YZ: Writing-review & editing, Software, Data curation. FK: Writing-review & editing.

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Competing interests

The authors declare that they have no competing interests.

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Code and data availability

The UpsFrac code is available on GitHub (https://github.com/chentao9330/UpsFrac, last access: 16 January 2024), and version 1.0 is archived on Zenodo (https://doi.org/10.5281/zenodo.14674083; Chen, 2025). The UpsFrac code is published under the GNU General Public License v3.0 (GPL-3.0 license). All input data in this study can be reproduced following the parameters and procedures described in this paper. The example input file used in this study can be found in the example folder of UpsFrac.

References

Almajid, M.M., Abu-Al-Saud, M.O., 2022. Prediction of porous media fluid flow using physics informed neural networks. Journal of Petroleum Science and Engineering 208, 109205. https://doi.org/10.1016/j.petrol.2021.109205

Andrews, B.J., Roberts, J.J., Shipton, Z.K., Bigi, S., Tartarello, M.C., Johnson, G., 2019. How do we see fractures? Quantifying subjective bias in fracture data collection. Solid Earth 10, 487–516. https://doi.org/10.5194/se-10-487-2019

Berre, I., Doster, F., Keilegavlen, E., 2018. Flow in Fractured Porous Media: A Review of Conceptual Models and Discretization Approaches. Transport in Porous Media 130, 215–236. https://doi.org/10.1007/s11242-018-1171-6

Bonnet, E., Bour, O., Odling, N.E., Davy, P., Main, I., Cowie, P., Berkowitz, B., 2001. Scaling of fracture systems in geological media. Reviews of Geophysics 39, 347–383. https://doi.org/10.1029/1999rg000074

Borghini, L., Striglio, G., Bacchiani, G., La Bruna, V., Balsamo, F., Bonini, L., Bezerra, F.H.R., 2024. Fracture analyser: a Python toolbox for the 2D analysis of fracture patterns. https://doi.org/10.3301/ijg.2024.16

Chen, T., 2025. Open-source software for integrating modelling and upscaling permeability for fractured porous rocks: UpsFrac. Zenodo. https://doi.org/10.5281/zenodo.14674083

Chen, T., Clauser, C., Marquart, G., Willbrand, K., Büsing, H., 2016. Modeling anisotropic flow and heat transport by using mimetic finite differences. Advances in Water Resources 94, 441–456. https://doi.org/10.1016/j.advwatres.2016.06.006

https://doi.org/10.5194/egusphere-2025-36
Preprint. Discussion started: 24 March 2025

Chen, T., Clauser, C., Marquart, G., Willbrand, K., Mottaghy, D., 2015. A new upscaling method for fractured porous media. Advances in Water Resources 80, 60–68. https://doi.org/10.1016/j.advwatres.2015.03.009

Cheng, Y., Wong, L.N.Y., 2018. Microscopic Characterization of Tensile and Shear Fracturing in Progressive Failure in Marble. Journal of Geophysical Research: Solid Earth 123, 204–225. https://doi.org/10.1002/2017JB014581

Cook, P.G., Love, A.J., Robinson, N.I., Simmons, C.T., 2005. Groundwater ages in fractured rock aquifers. Journal of Hydrology 308, 284–301. https://doi.org/10.1016/j.jhydrol.2004.11.005

Corral, Á., González, Á., 2019. Power Law Size Distributions in Geoscience Revisited. Earth and Space Science 6, 673–697. https://doi.org/10.1029/2018EA000479

Ebigbo, A., Lang, P.S., Paluszny, A., Zimmerman, R.W., 2016. Inclusion-Based Effective Medium Models for the Permeability of a 3D Fractured Rock Mass. Transport in Porous Media 113, 137–158. https://doi.org/10.1007/s11242-016-0685-z

Fadakar Alghalandis, Y., 2017. ADFNE: Open source software for discrete fracture network engineering, two and three dimensional applications. Computers & Geosciences 102, 1–11. https://doi.org/10.1016/j.cageo.2017.02.002

Fiori, A., Bellin, A., Cvetkovic, V., De Barros, F.P.J., Dagan, G., 2015. Stochastic modeling of solute transport in aquifers: From heterogeneity characterization to risk analysis. Water Resources Research 51, 6622–6648. https://doi.org/10.1002/2015WR017388

Ghassemi, A., 2012. A Review of Some Rock Mechanics Issues in Geothermal Reservoir Development. Geotech Geol Eng 30, 647–664. https://doi.org/10.1007/s10706-012-9508-3

Gong, L., Wang, J., Gao, S., Fu, X., Liu, B., Miao, F., Zhou, X., Meng, Q., 2021. Characterization, controlling factors and evolution of fracture effectiveness in shale oil reservoirs. Journal of Petroleum Science and Engineering 203, 108655. https://doi.org/10.1016/j.petrol.2021.108655

Gottron, D., Henk, A., 2021. Upscaling of fractured rock mass properties – An example comparing Discrete Fracture Network (DFN) modeling and empirical relations based on engineering rock mass classifications. Engineering Geology 294, 106382. https://doi.org/10.1016/j.enggeo.2021.106382

Gu, X., Rempe, D.M., Dietrich, W.E., West, A.J., Lin, T.-C., Jin, L., Brantley, S.L., 2020. Chemical reactions, porosity, and microfracturing in shale during weathering: The effect of erosion rate. Geochimica et Cosmochimica Acta 269, 63–100. https://doi.org/10.1016/j.gca.2019.09.044

Gudmundsson, A., 2011. Rock Fractures in Geological Processes. Cambridge University Press.

Hardebol, N.J., Bertotti, G., 2013. DigiFract: A software and data model implementation for flexible acquisition and processing of fracture data from outcrops. Computers & Geosciences 54, 326–336. https://doi.org/10.1016/j.cageo.2012.10.021

Healy, D., Rizzo, R.E., Cornwell, D.G., Farrell, N.J.C., Watkins, H., Timms, N.E., Gomez-Rivas, E., Smith, M., 2017. FracPaQ: A MATLABTM toolbox for the quantification of fracture patterns. Journal of Structural Geology 95, 1–16. https://doi.org/10.1016/j.jsg.2016.12.003

HosseiniMehr, M., Tomala, J.P., Vuik, C., Kobaisi, M.A., Hajibeygi, H., 2022. Projection-based embedded discrete fracture model (pEDFM) for flow and heat transfer in real-field geological formations with hexahedral corner-point grids. Advances in Water Resources 159, 104091. https://doi.org/10.1016/j.advwatres.2021.104091

Hyman, J.D., Aldrich, G., Viswanathan, H., Makedonska, N., Karra, S., 2016. Fracture size and transmissivity correlations: Implications for transport simulations in sparse three-dimensional discrete fracture networks following a truncated power law distribution of fracture size. Water Resources Research 52, 6472–6489. https://doi.org/10.1002/2016wr018806

Keilegavlen, E., Berge, R., Fumagalli, A., Starnoni, M., Stefansson, I., Varela, J., Berre, I., 2021. PorePy: an open-source software for simulation of multiphysics processes in fractured porous media. Comput Geosci 25, 243–265. https://doi.org/10.1007/s10596-020-10002-5

Keller, J., Rath, V., Bruckmann, J., Mottaghy, D., Clauser, C., Wolf, A., Seidler, R., Bücker, H.M., Klitzsch, N., 2020. SHEMAT-Suite: An open-source code for simulating flow, heat and species transport in porous media. SoftwareX 12, 100533. https://doi.org/10.1016/j.softx.2020.100533

Klimczak, C., Schultz, R.A., Parashar, R., Reeves, D.M., 2010. Cubic law with aperture-length correlation: implications for network scale fluid flow. Hydrogeology Journal 18, 851–862. https://doi.org/10.1007/s10040-009-0572-6

Kolditz, O., Bauer, S., Bilke, L., Böttcher, N., Delfs, J.O., Fischer, T., Görke, U.J., Kalbacher, T., Kosakowski, G., McDermott, C.I., Park, C.H., Radu, F., Rink, K., Shao, H., Shao, H.B., Sun, F., Sun, Y.Y., Singh, A.K., Taron, J., Walther, M., Wang, W., Watanabe, N., Wu, Y., Xie, M., Xu, W., Zehner, B., 2012. OpenGeoSys: an open-source initiative for numerical simulation of thermo-hydro-mechanical/chemical (THM/C) processes in porous media. Environmental Earth Sciences 67, 589–599. https://doi.org/10.1007/s12665-012-1546-x

Lang, P.S., Paluszny, A., Zimmerman, R.W., 2014. Permeability tensor of three-dimensional fractured porous rock and a comparison to trace map predictions. Journal of Geophysical Research: Solid Earth 119, 6288–6307. https://doi.org/10.1002/2014jb011027

Li, Z., Sherman, C.S., Reagan, M.T., Moridis, G.J., Morris, J.P., 2022. Effects of Heterogeneous Fracture Aperture on Multiphase Production from Shale Reservoirs. Transp Porous Med 144, 797–823. https://doi.org/10.1007/s11242-022-01841-0

Lie, K.-A., 2019. An Introduction to Reservoir Simulation Using MATLAB/GNU Octave: User Guide for the MATLAB Reservoir Simulation Toolbox (MRST). Cambridge University Press, Cambridge.

Liu, Z., Reynolds, A.C., n.d. History Matching an Unconventional Reservoir with a Complex Fracture Network.

MacQuarrie, K.T.B., Mayer, K.U., 2005. Reactive transport modeling in fractured rock: A state-of-the-science review. Earth-Science Reviews 72, 189–227. https://doi.org/10.1016/j.earscirev.2005.07.003

Marinos, Vassilis., Carter, Trevor.G., 2018. Maintaining geological reality in application of GSI for design of engineering structures in rock. Engineering Geology 239, 282–297. https://doi.org/10.1016/j.enggeo.2018.03.022

https://doi.org/10.5194/egusphere-2025-36
Preprint. Discussion started: 24 March 2025

Massart, B., Paillet, M., Henrion, V., Sausse, J., Dezayes, C., Genter, A., Bisset, A., 2010. Fracture characterization and stochastic modeling of the granitic basement in the HDR Soultz Project (France), in: Proceedings World Geothermal Congress 2010. Bali, Indonesia.

McDermott, C., Kolditz, O., 2006. Geomechanical model for fracture deformation under hydraulic, mechanical and thermal loads. Hydrogeol J 14, 485–498. https://doi.org/10.1007/s10040-005-0455-4

Mejia, C., Roehl, D., Rueda, J., Quevedo, R., 2021. A new approach for modeling three-dimensional fractured reservoirs with embedded complex fracture networks. Computers and Geotechnics 130, 103928. https://doi.org/10.1016/j.compgeo.2020.103928

Molnar, P., Anderson, R.S., Anderson, S.P., 2007. Tectonics, fracturing of rock, and erosion. Journal of Geophysical Research: Earth Surface 112. https://doi.org/10.1029/2005JF000433

Myers, T., 2012. Potential Contaminant Pathways from Hydraulically Fractured Shale to Aquifers. Groundwater 50, 872–882. https://doi.org/10.1111/j.1745-6584.2012.00933.x

Neuman, S.P., 2005. Trends, prospects and challenges in quantifying flow and transport through fractured rocks. Hydrogeology Journal 13, 124–147.

Oda, M., 1985. Permeability tensor for discontinuous rock masses. Géotechnique 35, 483–495. https://doi.org/10.1680/geot.1985.35.4.483

Odling, N.E., Roden, J.E., 1997. Contaminant transport in fractured rocks with significant matrix permeability, using natural fracture geometries. Journal of Contaminant Hydrology 27, 263–283. https://doi.org/10.1016/S0169-7722(96)00096-4

Olson, J.E., 2003. Sublinear scaling of fracture aperture versus length: An exception or the rule? Journal of Geophysical Research: Solid Earth 108. https://doi.org/10.1029/2001jb000419

Ovaskainen, N., 2023. fractopo: A Python package for fracture network analysis. Journal of Open Source Software 8, 5300. https://doi.org/10.21105/joss.05300

Palamakumbura, R., Krabbendam, M., Whitbread, K., Arnhardt, C., 2020. Data acquisition by digitizing 2-D fracture networks and topographic lineaments in geographic information systems: further development and applications. Solid Earth 11, 1731–1746. https://doi.org/10.5194/se-11-1731-2020

Rajeh, T., Ababou, R., Marcoux, M., Cañamon, I., 2019. Fast Upscaling of the Hydraulic Conductivity of Three-Dimensional Fractured Porous Rock for Reservoir Modeling. Math Geosci 51, 1037–1074. https://doi.org/10.1007/s11004-019-09785-w

Renard, P., Ababou, R., 2022. Equivalent Permeability Tensor of Heterogeneous Media: Upscaling Methods and Criteria (Review and Analyses). Geosciences 12, 269. https://doi.org/10.3390/geosciences12070269

Sandve, T.H., Berre, I., Nordbotten, J.M., 2012. An efficient multi-point flux approximation method for Discrete Fracture–Matrix simulations. Journal of Computational Physics 231, 3784–3800. https://doi.org/10.1016/j.jcp.2012.01.023

Schultz, R.A., Soliva, R., 2012. Propagation energies inferred from deformation bands in sandstone. Int J Fract 176, 135–149. https://doi.org/10.1007/s10704-012-9730-2

https://doi.org/10.5194/egusphere-2025-36
Preprint. Discussion started: 24 March 2025

Srinivasan, G., Hyman, J.D., Osthus, D.A., Moore, B.A., O'Malley, D., Karra, S., Rougier, E., Hagberg, A.A., Hunter, A., Viswanathan, H.S., 2018. Quantifying Topological Uncertainty in Fractured Systems using Graph Theory and Machine Learning. Sci Rep 8, 11665. https://doi.org/10.1038/s41598-018-30117-1

Vermilye, J.M., Scholz, C.H., 1995. Relation between vein length and aperture. Journal of Structural Geology 17, 423–434. https://doi.org/10.1016/0191-8141(94)00058-8

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, e2021RG000744. https://doi.org/10.1029/2021RG000744

Wang, Q., Zhang, L., Yu, Q., Li, H., 2023. Existence analysis of hydraulic conductivity representative elementary volume in fractured rocks based on three-dimensional discrete fracture network method. Computers and Geotechnics 164, 105829.

Welch, M. J., Lüthje, M., Oldfield, S. J., 2022. DFN Generator v2. 0: A new tool to model the growth of large-scale natural fracture networks using fundamental geomechanics. Geoscientific Model Development Discussions, 2022, 1-42.

Weismüller, C., Prabhakaran, R., Passchier, M., Urai, J.L., Bertotti, G., Reicherter, K., 2020. Mapping the fracture network in the Lilstock pavement, Bristol Channel, UK: manual versus automatic. Solid Earth 11, 1773–1802. https://doi.org/10.5194/se-11-1773-2020

Xu, C., Dowd, P., 2010. A new computer code for discrete fracture network modelling. Computers & Geosciences 36, 292–301. https://doi.org/10.1016/j.cageo.2009.05.012

Xue, K., Zhang, Z., Zhong, C., Jiang, Y., Geng, X., 2022. A fast numerical method and optimization of 3D discrete fracture network considering fracture aperture heterogeneity. Advances in Water Resources 162, 104164. https://doi.org/10.1016/j.advwatres.2022.104164

Yan, M., Huang, C., Bienstman, P., Tino, P., Lin, W., Sun, J., 2024. Emerging opportunities and challenges for the future of reservoir computing. Nat Commun 15, 2056. https://doi.org/10.1038/s41467-024-45187-1

Yan, X., Lin, J., Wang, S., Zhang, Z., Liu, P., Sun, S., Yao, J., Zhang, K., 2024. Physics-informed neural network simulation of two-phase flow in heterogeneous and fractured porous media. Advances in Water Resources 189, 104731. https://doi.org/10.1016/j.advwatres.2024.104731

Zijl, W., Stam, J.M.T., 1992. Modeling permeability in imperfectly layered porous media. I. Derivation of block-scale permeability tensor for thin grid-blocks. Math Geol 24, 865–883. https://doi.org/10.1007/BF00894656

Zoback, M.D., Barton, C.A., Brudy, M., Castillo, D.A., Finkbeiner, T., Grollimund, B.R., Moos, D.B., Peska, P., Ward, C.D., Wiprut, D.J., 2003. Determination of stress orientation and magnitude in deep wells. International Journal of Rock Mechanics and Mining Sciences, Special Issue of the IJRMMS: Rock Stress Estimation ISRM Suggested Methods and Associated Supporting Papers 40, 1049–1076. https://doi.org/10.1016/j.ijrmms.2003.07.001