Simulating flow, transport and hydrogeochemical processes within fracture networks

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Abstract

Modelling physical processes such as flow and transport within a fracture network can be challenging, both conceptually and numerically. A typical approach is to upscale the properties of the network onto a regular grid of elements, which is then used to simulate the required physical processes. However, this method can be inaccurate if not carefully applied. For example, when most of the flow passes through a few choke points in the network, upscaling may introduce extra connectivity that is not present in the original network. The ConnectFlow software package has an alternative method for representing fracture networks, whereby the fractures are explicitly modelled as a network of intersecting two dimensional planes. The algorithms within ConnectFlow are very efficient, allowing millions of separate fractures to be simulated, each discretised using hundreds of finite elements. Here we present recent updates to this functionality: 1) to allow the advection-diffusion equation to be solved for multiple solute species (which is fully coupled to the pressure solution via the buoyancy term in Darcy's equation); 2) to model the diffusion of solutes into the pore space of the surrounding rock (i.e. matrix diffusion); and 3) to carry out chemical reactions between solutes and minerals (which coat the fractures and/or the rock pores) using an interface to the IPhreeqc library. The ConnectFlow algorithms have also been parallelised to improve the tractability of this new functionality. This implementation represents a significant step forward in capability that allows groundwater flow, transport and hydrogeochemical reactions to be properly represented in the context of structurally constrained fractured bedrock. This has a wide range of potential applications, particularly for future safety assessments of nuclear waste facilities. Example calculations are presented for the Onkalo disposal facility in Olkiluoto, Finland, and the proposed Swedish repository for long-lived waste, SFL.

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Simulating flow, transport and hydrogeochemical processes within fracture networks

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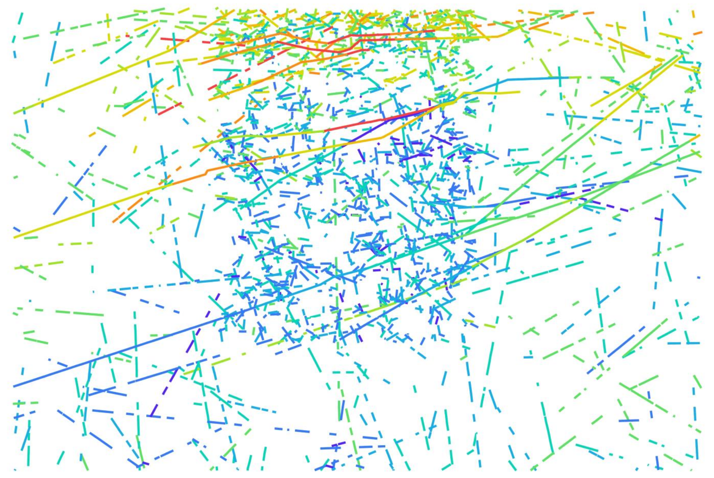
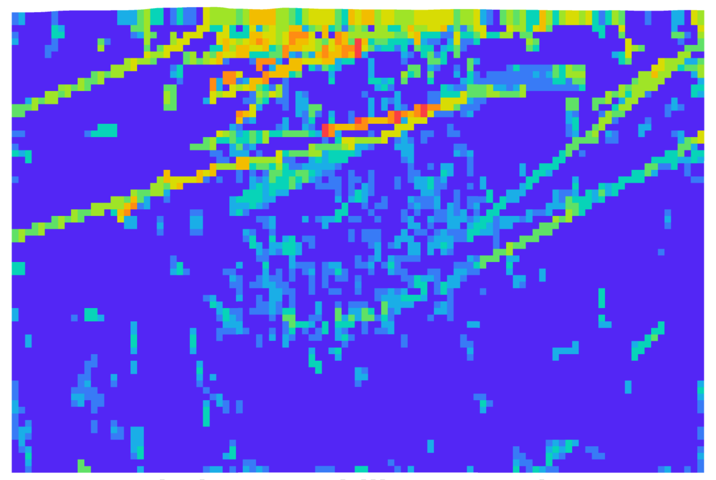
Introduction

Modelling physical processes such as flow and transport within a fracture network is challenging, both conceptually and numerically. A typical approach is to upscale the properties of the network onto a regular grid of elements. This is then used to simulate the required physical processes.



Fracture transmissivity for a vertical slice through a model of Olkiluoto Island.



Upscaled permeability – note how some of the fractures are agglomerated into the same cell – potential for unphysical connectivity

However, this method can be inaccurate if not carefully applied. For example, if the flow passes through a few choke points in the network, upscaling may introduce extra connectivity not present in the original network. Work on brittle fracture zones has also shown upscaling can be less accurate when the orientation of fractures is focused in a single direction and the resulting permeability tensors are anisotropic.

The ConnectFlow [1] software package has an alternative method for representing discrete fracture networks (DFNs): the fractures are explicitly modelled as a network of intersecting two dimensional planes. The algorithms are efficient, allowing millions of fractures to be simulated, each discretised using hundreds of finite elements. Here we present recent updates to this functionality:

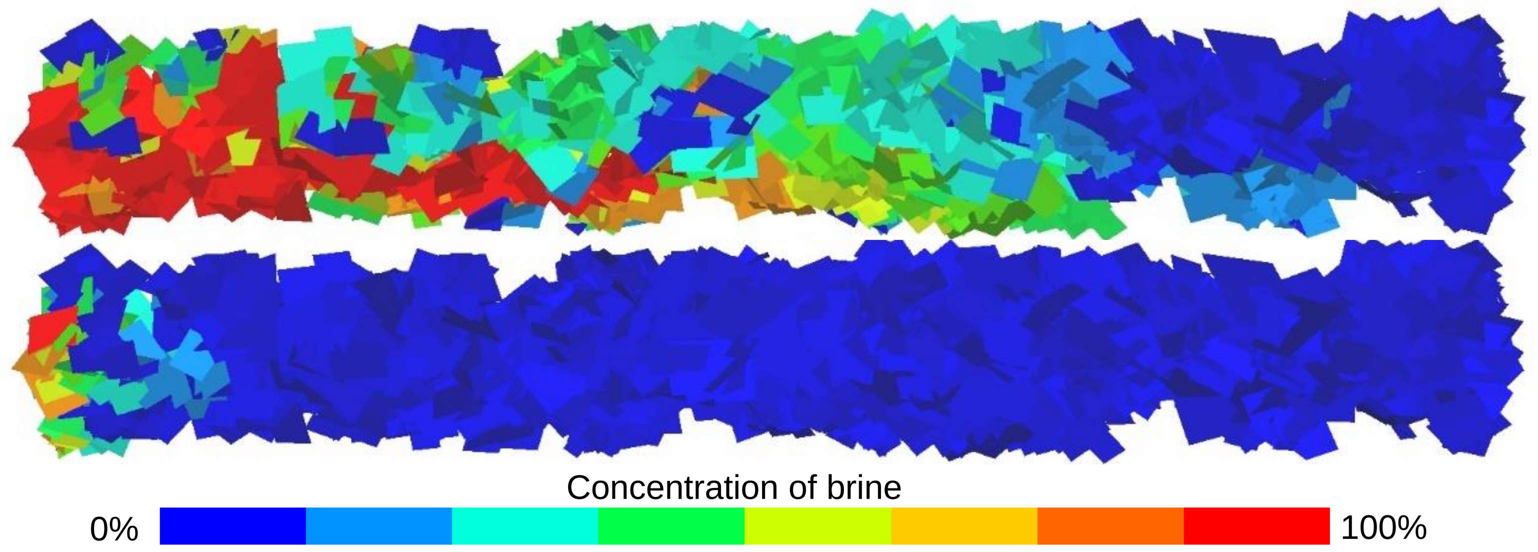
- solutions to the advection-diffusion equation for multiple solute species (including buoyancy);
- to model the diffusion into the pore space of the surrounding rock (rock matrix diffusion or RMD);
- to carry out chemical reactions between solutes and minerals;
- the ConnectFlow algorithms have also been parallelised to improve the tractability.

This is a significant advance, allowing groundwater flow, transport and hydrogeochemical reactions to be represented explicitly in fractured bedrock. Examples for the ONKALO disposal facility in Olkiluoto, Finland, and the proposed Swedish repository for long-lived waste, SFL are presented.

DFN Modelling in ConnectFlow

ConnectFlow's DFN module explicitly represents individual 2D rock fractures intersecting with each other in 3D space using their own geometric and hydraulic properties. The module has been developed over a period of 25 years and been extensively verified in international comparison exercises. Its efficiency has enabled flow calculations for SFL and Olkiluoto models involving millions of individually modelled fractures.

ConnectFlow has recently been updated to allow the solution of transient solute transport equation for multiple species. Concentrations are fully coupled to the pressure solution via the buoyancy term in Darcy's equation. Rock matrix diffusion can be included [2].



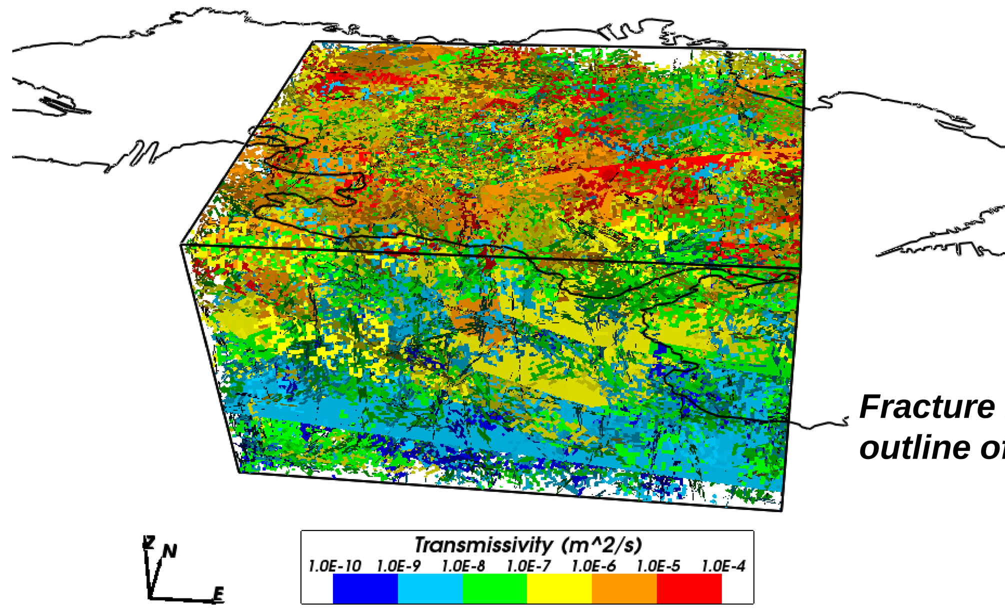
Simple example with brine transported left to right along a column of random fractures. The top figure has no RMD. The bottom figure has RMD which retards the transport.

Additionally, chemical reactions between solutes and minerals (which coat the fractures and/or the rock pores) are calculated via an interface to the Phreeqc [3] library (iPhreeqc).

The example on the left demonstrates a simple example of salt transport from left to right along several randomly distributed fractures with and without matrix diffusion.

Meteoric water intrusion at Olkiluoto Island

The ONKALO is a deep geological repository for the final disposal of spent nuclear fuel. This is the first such repository in the world. Currently under construction, the ONKALO is located at Olkiluoto Island, on the west coast of Finland. The ONKALO is located within a fractured crystalline bedrock. We have prepared a demonstration model that simulates the ingress of meteoric water. Over time this water displaces saline water in the upper bedrock.



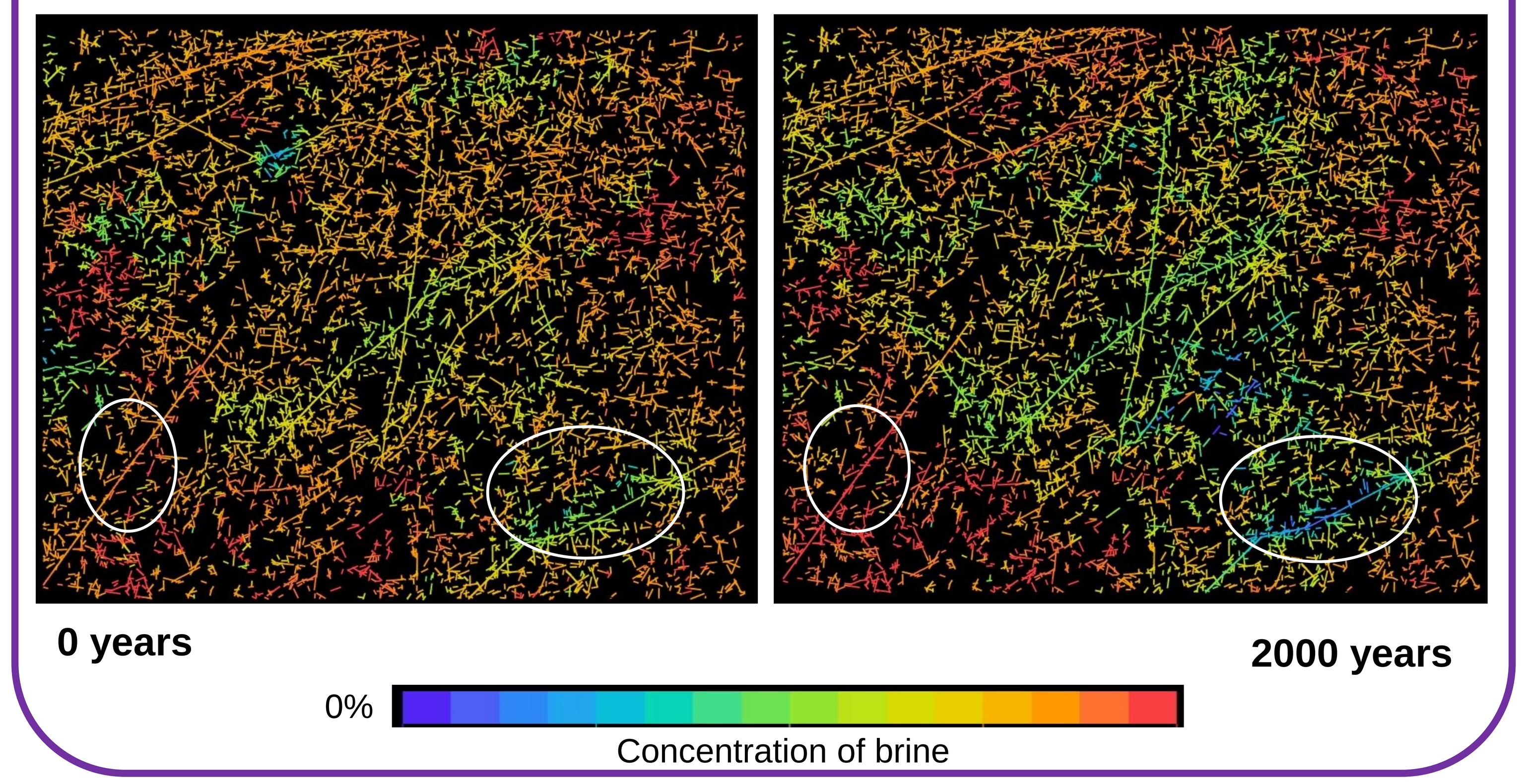
Fracture network and outline of Island

Transient 3D Simulation of an island scale model of Olkiluoto

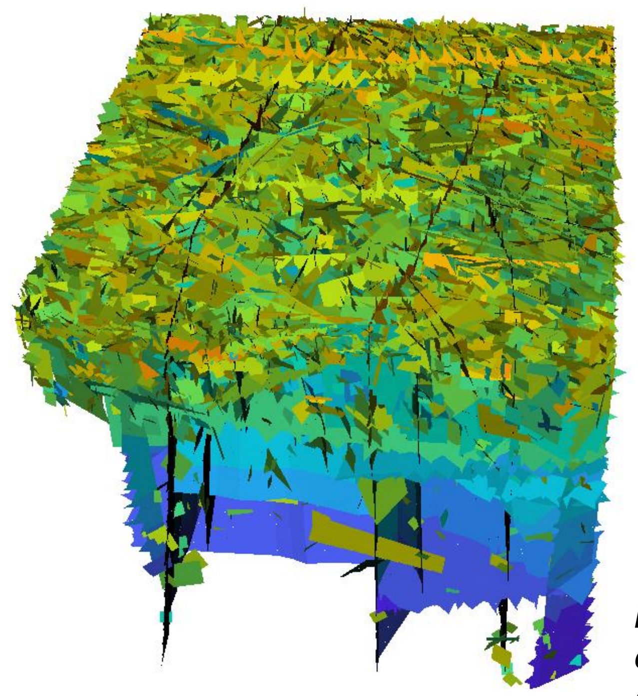
- Simulation domain is 2.7 x 3.0 km and 1.4 km deep. All fractures bigger than 20m included (538,000 fractures)
- Simulation is run for 2000 years
- ONKALO centred at a depth of -410 masl
- Initial condition has increasing salinity with depth
- Rock matrix diffusion included
- Meteoric water penetrates at the top and percolates downward
- Relatively saline water at repository depth is gradually displaced and diluted by surface waters over thousands of years

Results (see slices below):

- Transport occurs more quickly in larger fractures
- Smaller fractures are affected over longer timescales
- In some locations saline water is displaced by meteoric water from above. In others, water is displaced by more saline water from below.



Reactive transport modelling at SFL



Fracture network – lighter colours show bigger apertures

SFL is SKB's proposed disposal facility of long-lived low and intermediate level nuclear waste. We have produced a demonstration model showing how ingress of meteoric water might reach repository depth.

Transient 3D Simulation of Laxemar (example location).

- Simulation domain is a 2.2 km sided cube
- Fractures bigger than 50m included
- SFL assumed depth centred at -490 masl
- 2000 year transient calculation
- Six solute species: Na, Cl, C, Ca, O, H
- Calcite equilibrium reaction included:

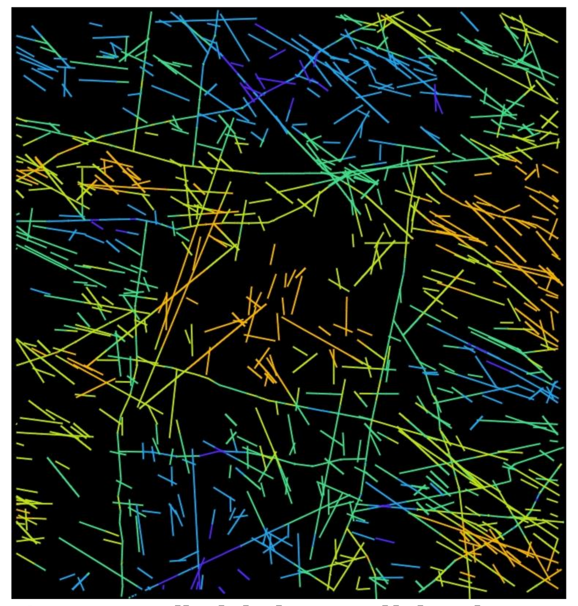
$$CaCO_3 + H_2CO_3 = Ca^{+2} + 2HCO_3^{-1}$$

- Rock matrix diffusion included

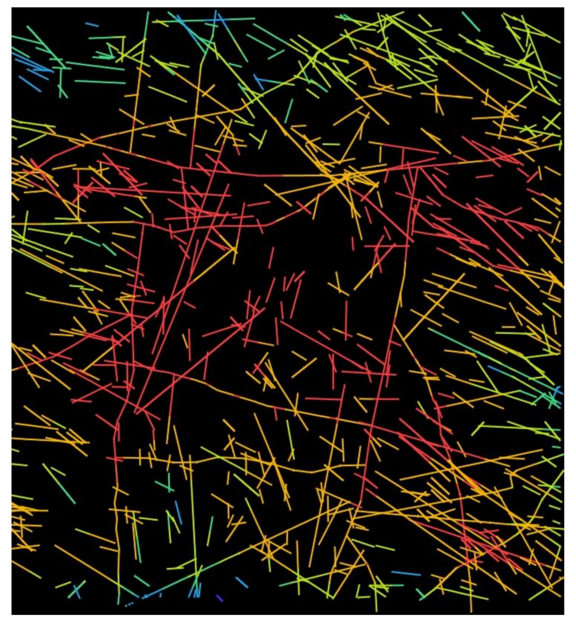
Results

- Images to right are slices at -490masl through DFN, coloured by carbon concentration
- Water at these depths contain low concentrations of inorganic carbon (first slice)
- Over time this is displaced by water from above with higher carbon concentrations (second slice)
- Calcite reactions (when included) slow the rate at which carbon rich water descends (final slice)

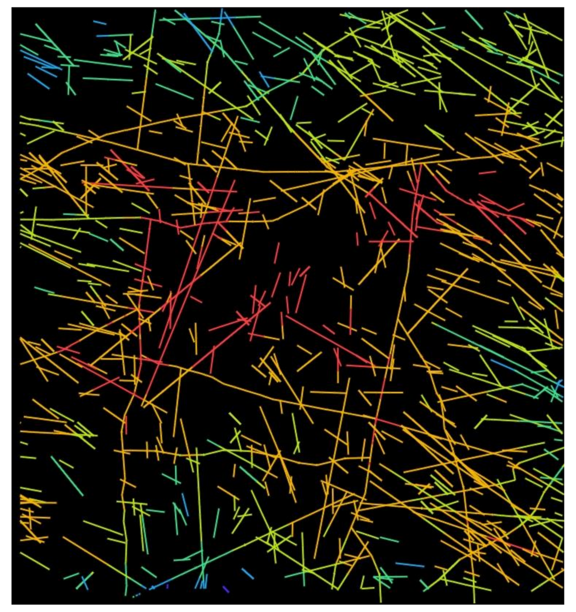
Mass fraction of carbon (for plots to right)



0 years (initial condition)



2000 years without reactions



2000 years with reactions

Conclusions

- Repositories in Sweden and Finland will be situated in fractured crystalline rock. Understanding hydrogeochemical processes is key to ascertaining their safety. These processes are best understood by representing the fractures as a network of intersecting 2D structures rather than a continuum.
- ConnectFlow now has a full implementation of multicomponent salt transport for DFNs. Chemical reactions can be included and/or RMD. Parallelisation has allowed more complex models to be simulated.

[1] **Wood. ConnectFlow Technical Reference.** www.connectflow.com/resources/docs/conflow_technical.pdf
[2] **Hartley L & Joyce S.** Approaches and algorithms for groundwater flow modeling in support of site investigations and safety assessment of the Forsmark site, Sweden. Journal of Hydrology, Volume 500, 13 Sept 2013, Pages 200-216.
[3] **Parkhurst D L and Appelo C, 1999.** User's guide to PHREEQC (Version 2)—A computer program for speciation, batch-reaction, one-dimensional transport, and inverse geochemical calculations:.U.S. Geological Survey Water-Resources Investigations Report 99–4259.