High Performance Computing: an appealing solution for assessing radionuclide transport in fractured media at a grain-pore scale

1. Motivation

LTD55D experiment at Åspö (Sweden) [1] “...predictive modelling was made for the tracer penetration profiles(...). Regardless of the chosen parameters, the discrepancies between the modelled and observed profiles were more pronounced than the similarities”

“The heterogeneous nature of the rock matrix, in terms of both the microporous network and mineral surfaces available for sorption, has been qualitatively offered as an explanation for the discrepancy”

2. A synthetic fracture-rock matrix model

- Grains (i.e. fracture-free volumes) are assumed to contain a given amount of biotite plus other chemically inert solid phases and a very low amount of pore space (i.e., intra-granular porosity).
- Inter-granular regions are assumed to consist of a higher amount of pore space (i.e., inter-granular porosity) and chemically inert solid phases.
- Each grid cell of the matrix is identified as being either part of a grain or an inter-granular region.
- Alternative equivalent model -> biotite is assumed to be homogeneously distributed in the matrix, being the total volume of biotite the same for the two models (i.e. same amount of cation exchange sites).
- 1,243,008 elements are used to represent the fracture, while 51,584,832 elements constitute the rock matrix (i.e. a total of 52,827,840 rectangular cuboids) = discretization in the order of a few micrometers

3. Scalability Test Results

- Cesium is injected along one of the boundaries of the fracture and:
  - moves along the fracture driven by advection
  - diffuses into the matrix where it might eventually be sorbed onto biotite surfaces

- A total of 3.5M core-hours have been spent with each simulation run on an average of 8,192 cores.
- A total of 32K calculation time steps have been calculated.

4. Results

- The calculations were solved using PFLOTRAN [3], which was run on the supercomputer JUQUEEN at the Jülich Supercomputing Centre [4].
- A custom-made interface (IDP) [5] was used to extract the Darcy’s velocities computed by Darcy Tools [6] at cell faces, which then were used as input for PFLOTRAN

References

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