# Nanoparticle migration in a natural granite fracture

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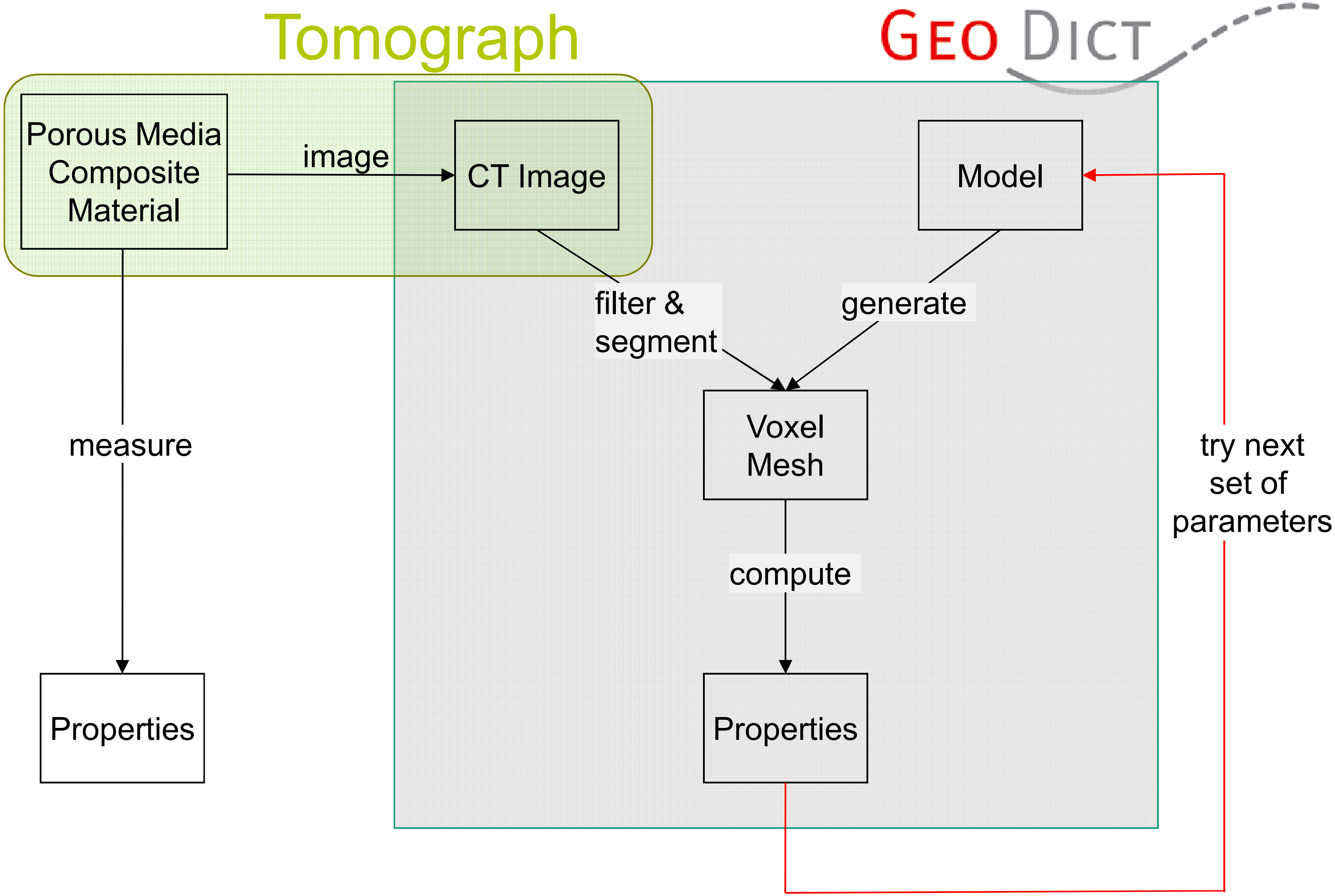
# Compute Material Properties with GeoDict

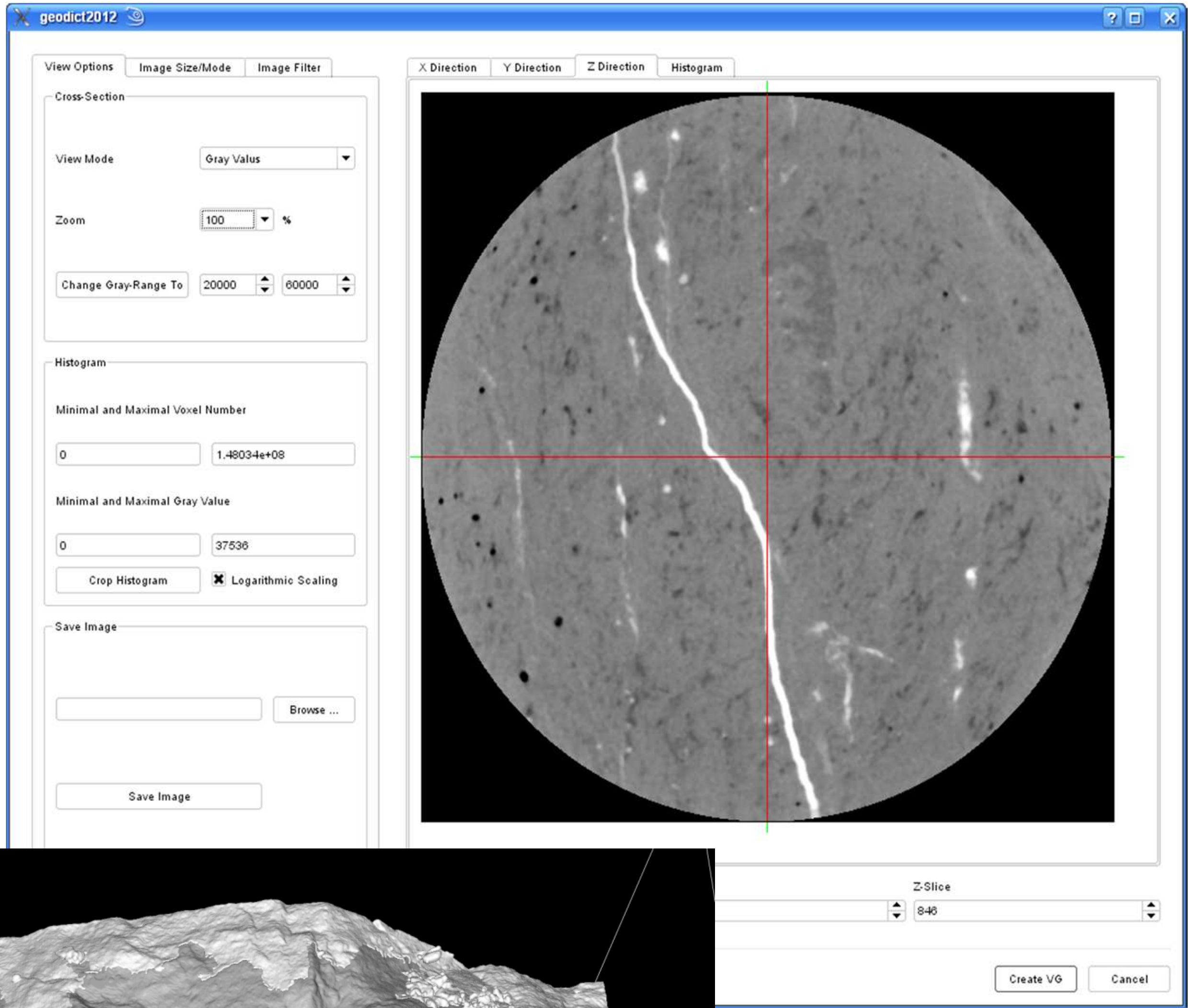


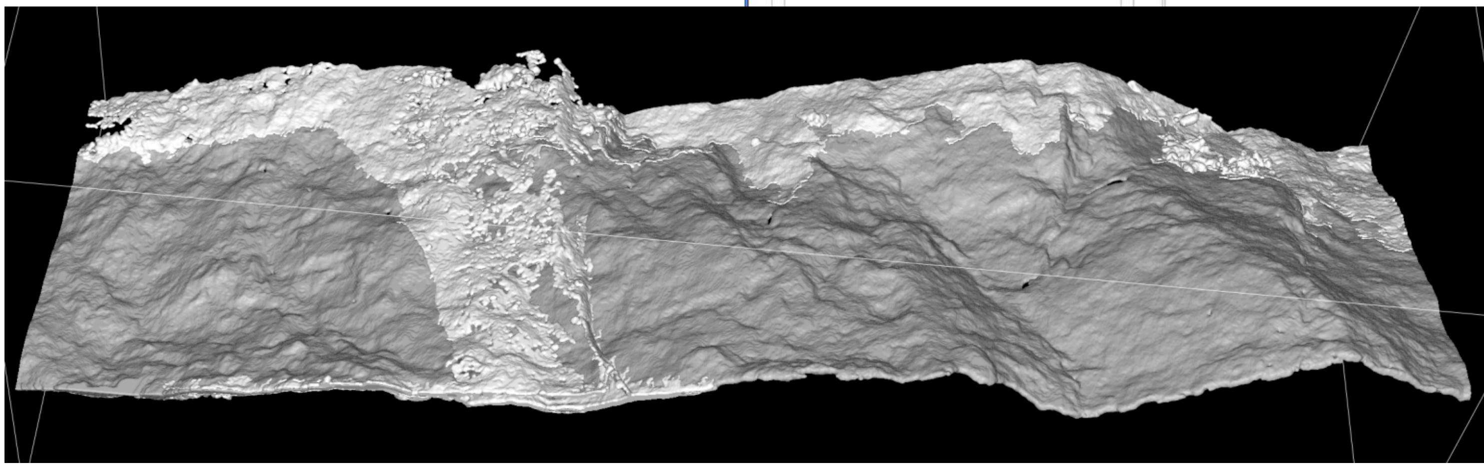
# The Tomogram

CT of a granite fracture:

- resolution of 80 µm
- segmented: pores, porous material, solid
- size 631x631x1691voxel

*(by F. Enzmann et al at the University of Mainz, Institute for Geosciences)*





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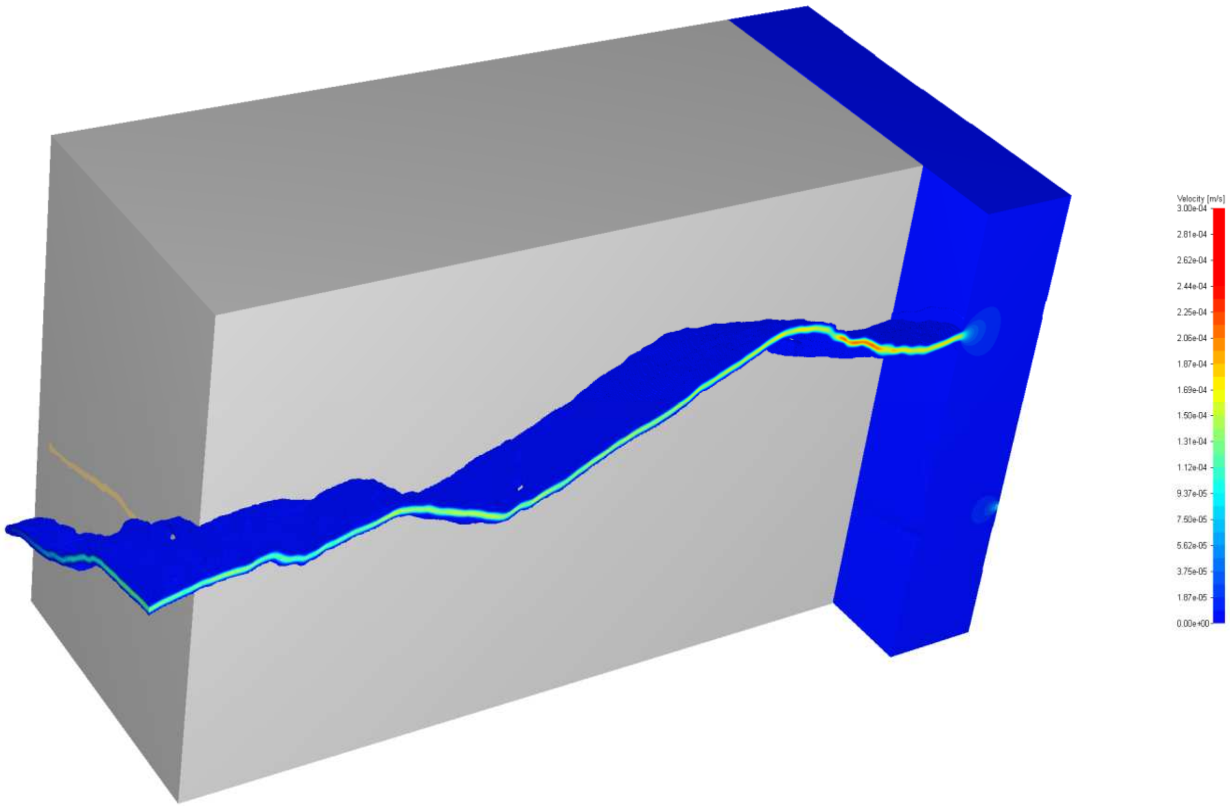
# The Flow Simulation




incompressible stationary Navier–Stokes equation:

$$-\mu \Delta u + \nabla p + \rho u \Delta u = 0$$

$$-\mu \Delta u + \nabla p = 0$$

- finite volume solver (EFV in GeoDict
- method is optimized for large voxel grids
- porous material is viewed as solid

the computational costs for 631 x 631 x 1800 voxels:
8 processes on a 12-core desktop machine, 72 GB RAM, 4 h simulation time

flow simulation was performed for water at 20°C, flow rate 66.8 µL/min



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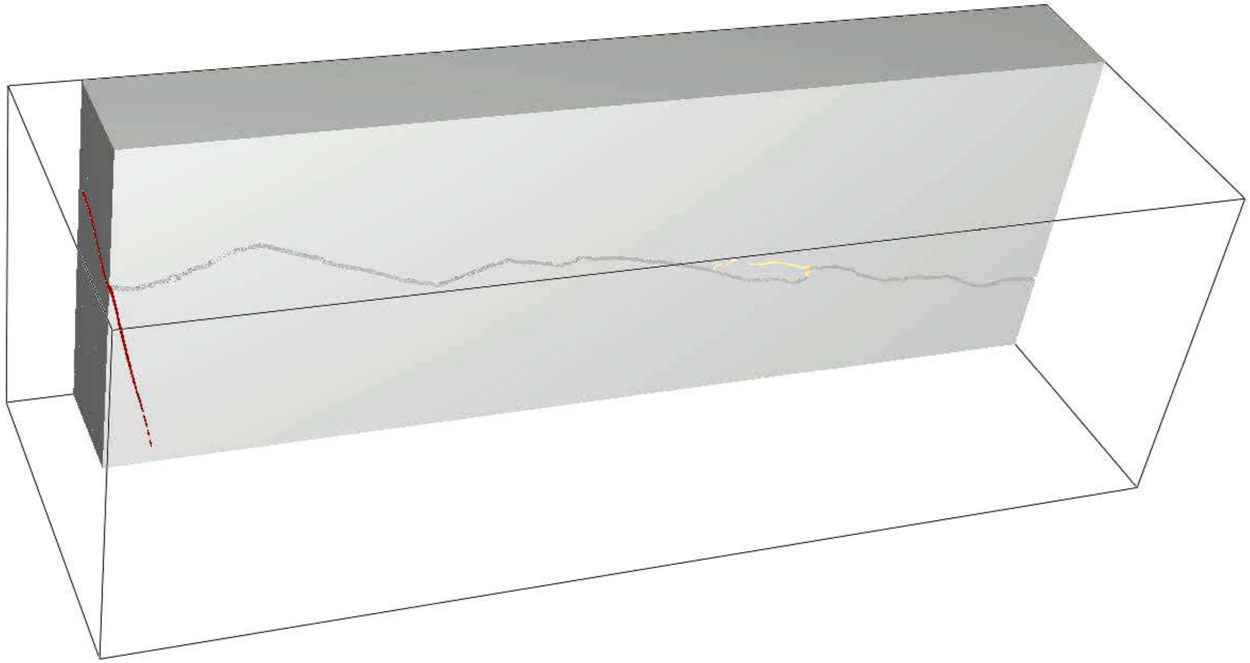
# The Transport Properties

**particle properties:**

- diameter 12 nm
- density 4000 kg/m3
- no chemical processes
- diffusion

=> simulation refracts the impact of fracture geometry on mass transport



**interaction model**:
particle hitting the fracture walls bounce, no energy-loss (sieving model GeoDict)

transport simulations => breakthrough curves



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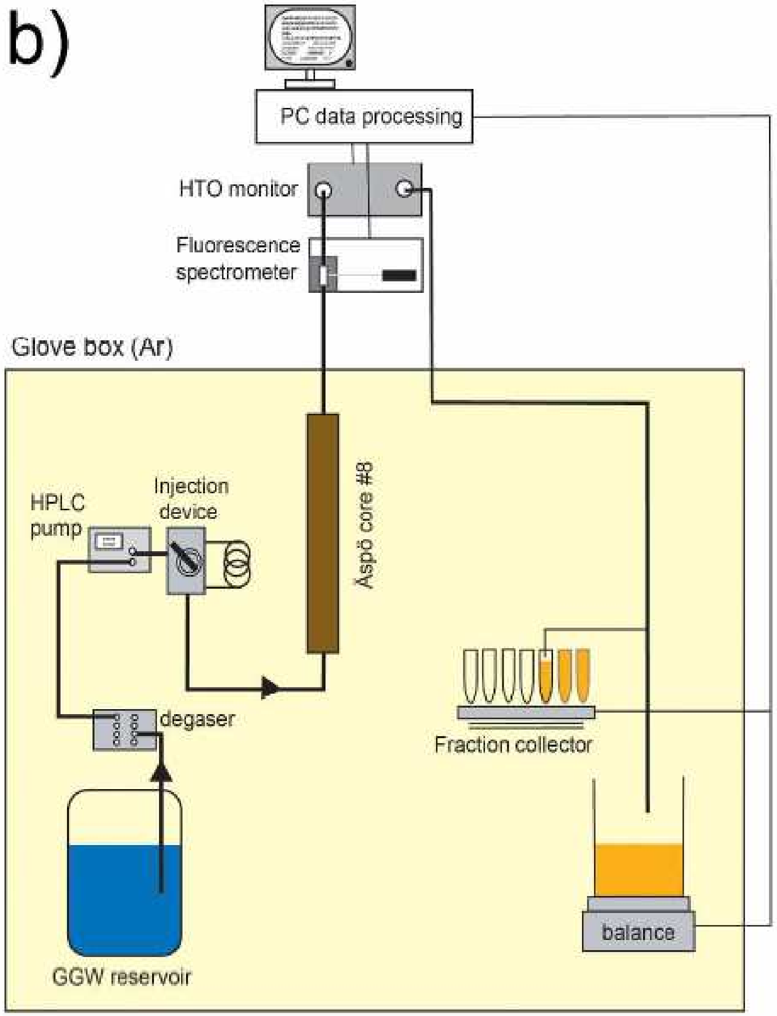
# Column Migration Experiment

a)

b)




*the nanoparticle (quantum dots) transport is experimentally realized by means of column migration experiments at the KIT, Institute for Nuclear Waste Disposal*

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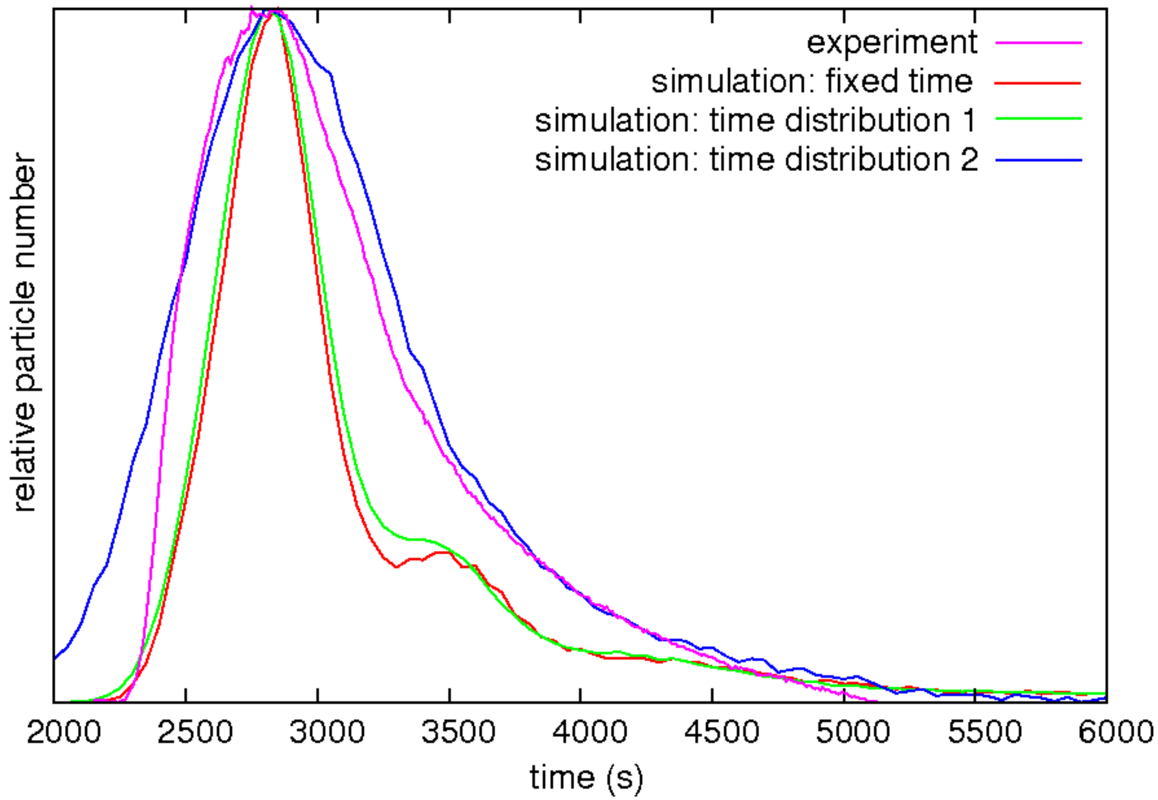
# Break-Through Curves

**simulation:**
varying starting times, particle numbers

red: 100,000 particles, fixed time

green: 1,000,000 particles, Gaussian distributed start times, standart deviation 100 sec

blue: 100,000 particles, standart deviation 300 sec




**experiment:** 66.8 µL/min, exact times and positions of particles entering the fracture unknown

=> changing start times the simulation matches the experimental result very well

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# Conclusions

**3D tomogram of a granite fracture**:

- compute flow / transport properties (GeoDict software)
- simulation agree very well with corresponding experimental results

**variations of the workflow:**

- different particle properties and start position
- different model for the interaction between rock and particle
- solve Stokes equation (less memory / run time) or the Stokes-Brinkmann equation (porous regions)
- calculate e.g. pore size distributions, elastic properties, saturation-dependent relative permeability, diffusion properties and conductivity

# Thank You!

Geometry generator,
property predictor and
virtual material
designer

www.geodict.com