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Setup of realistic large scale models

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Outline

- Short Problem description
- Grid: Workflow Petrel – Dumux
- Representation of fault zones
- Calibration: ITough2 and Dumux

Short Problem Description

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Motivation

- Deep Saline aquifers are an option for the storage of CO2 or the disposal of waste water
- The injection of fluids causes an increase in pressure reaching far beyond the radius of the plume of the injected fluid
- Fault zones, salt wall flanks or holes in the Rupelian Clay are possible pathways for the vertical migration of displaced brine in the North German Basin
- Displaced brine and contaminants from the deep subsurface may threaten water supply from groundwater
- This work was done in context of the CO2BRIM project

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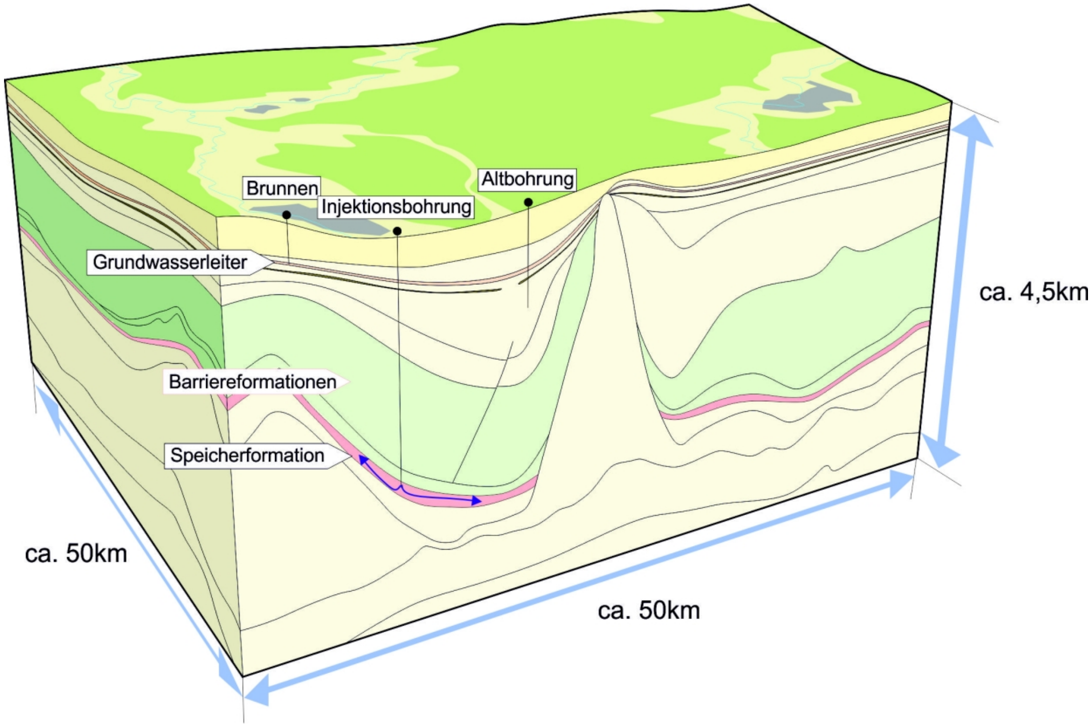
Case Study: Realistic CO2 Storage Site

- Application on a realistic scenario in the NGB
- Domain for CO2 injection contains a salt wall



Grid: Workflow Petrel – Dumux

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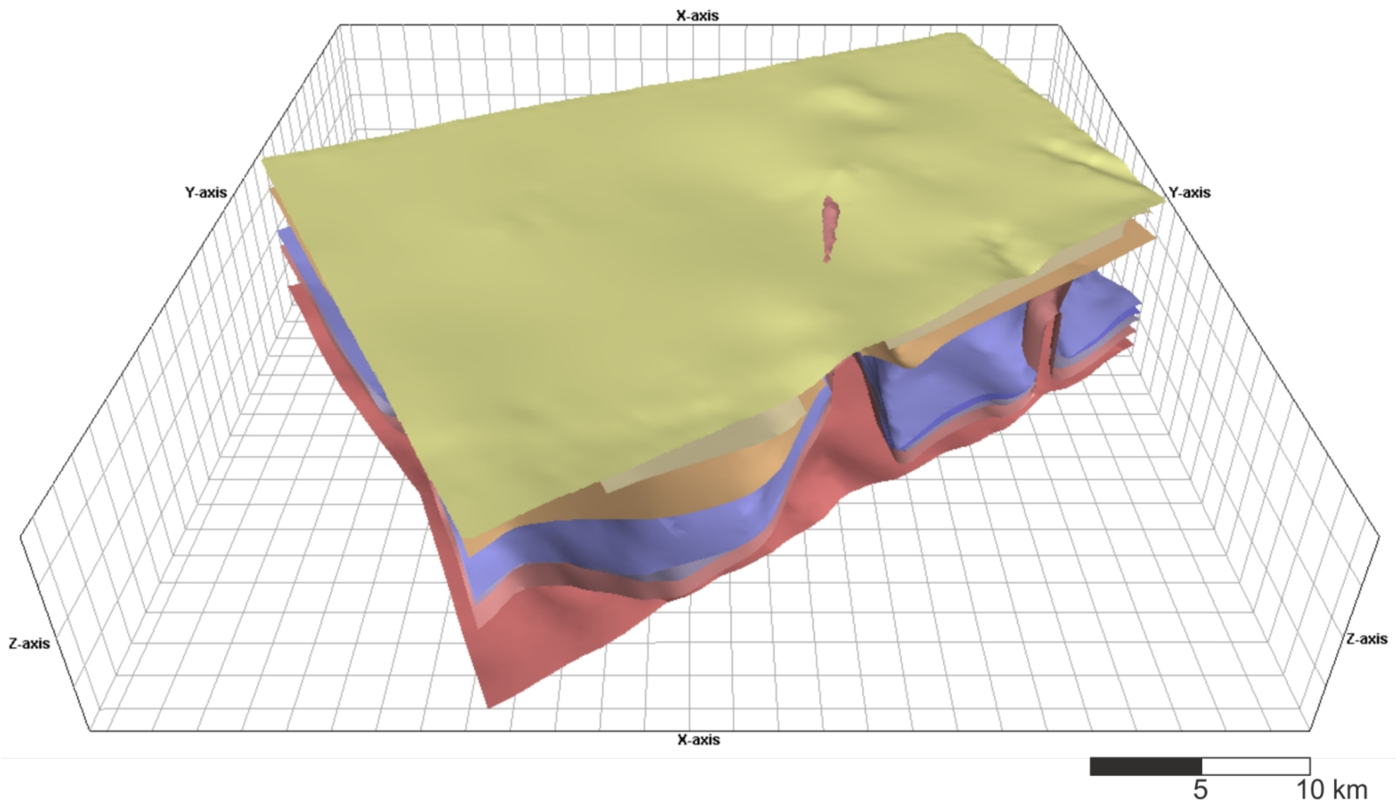
Geological layers

Bundesanstalt für Geowissenschaften und Rohstoffe



Injection layer and salt wall

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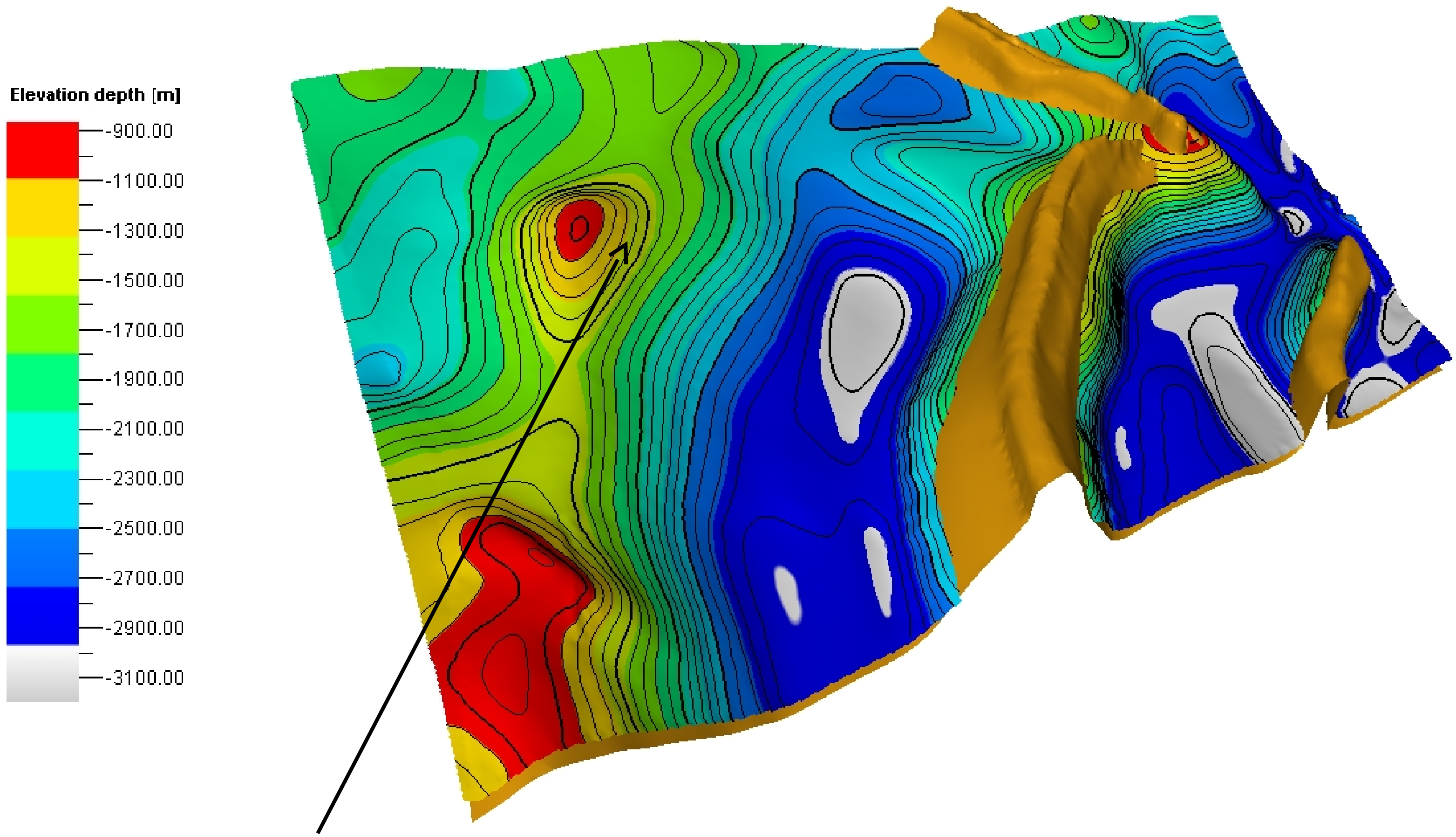
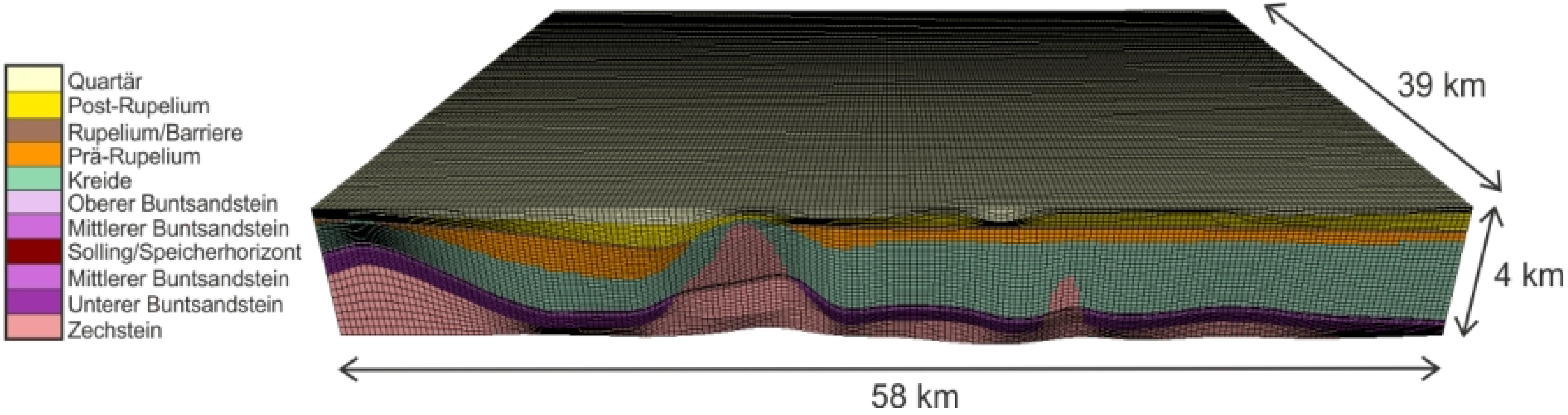


Injection point at ca. 1500 m depth
at the flank of the anticline

Grid

Bundesanstalt für Geowissenschaften und Rohstoffe

- Construction of a conforming 3D structural model with 11 geological layers
- Hexahedron Grid
- Lateral resolution 300m x 300m
- Vertical resolution 10m – 300m
- Nodes ~ 1.5 Million



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Workflow

- Use Petrel to create a conforming Hexahedron grid (no degenerated elements!)
- Export the coordinates and parameters to ascii files (*.GRDECL format)
- Install dune-cornerpoint module
- Use the converter *grdecl2vtu.cpp* and modify it by including and calling the *dgfwriter.hh* from dune-grid
- Adding material parameters for elements or nodes requires further modifications in *grdecl2vtu.cpp* and *dgfwriter.hh*
- Call *./grdecl2vtu grid.GRDECL*

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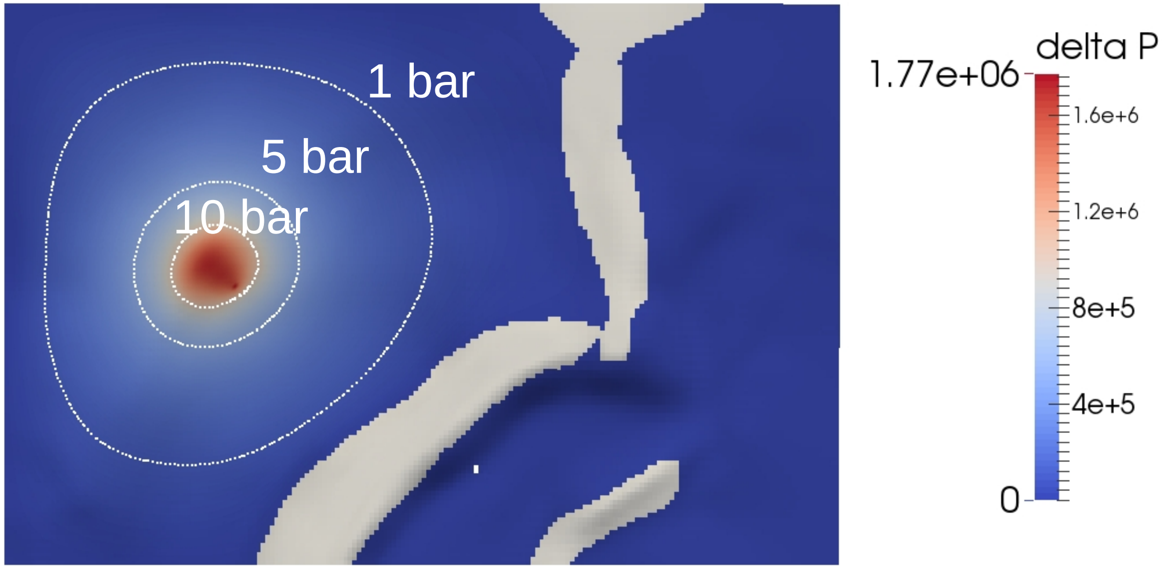
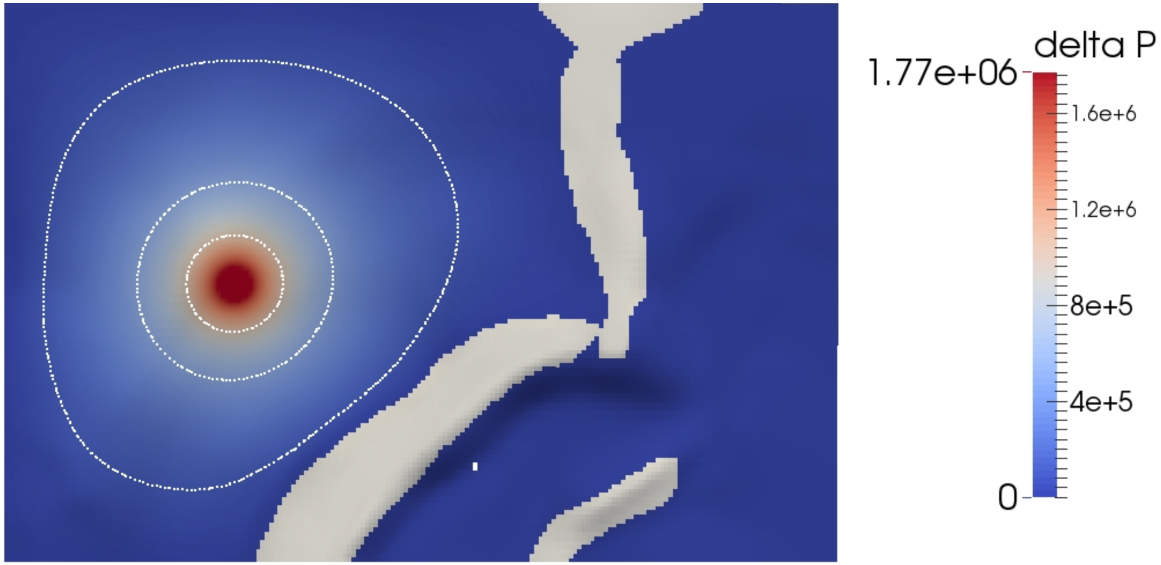
2 phase flow vs 1 phase flow

2 phase flow



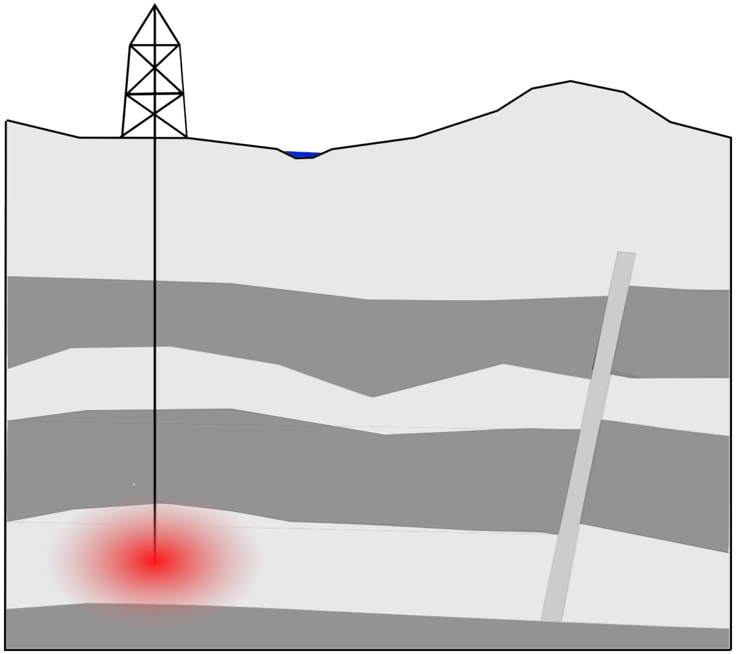
1 phase flow



Representation of fault zones

Fault zone

- Vertical discontinuity in layered system
- Can be conduit or barrier for flow
- Thickness up to 100 m
- Resolving the fault zone usually requires refinement



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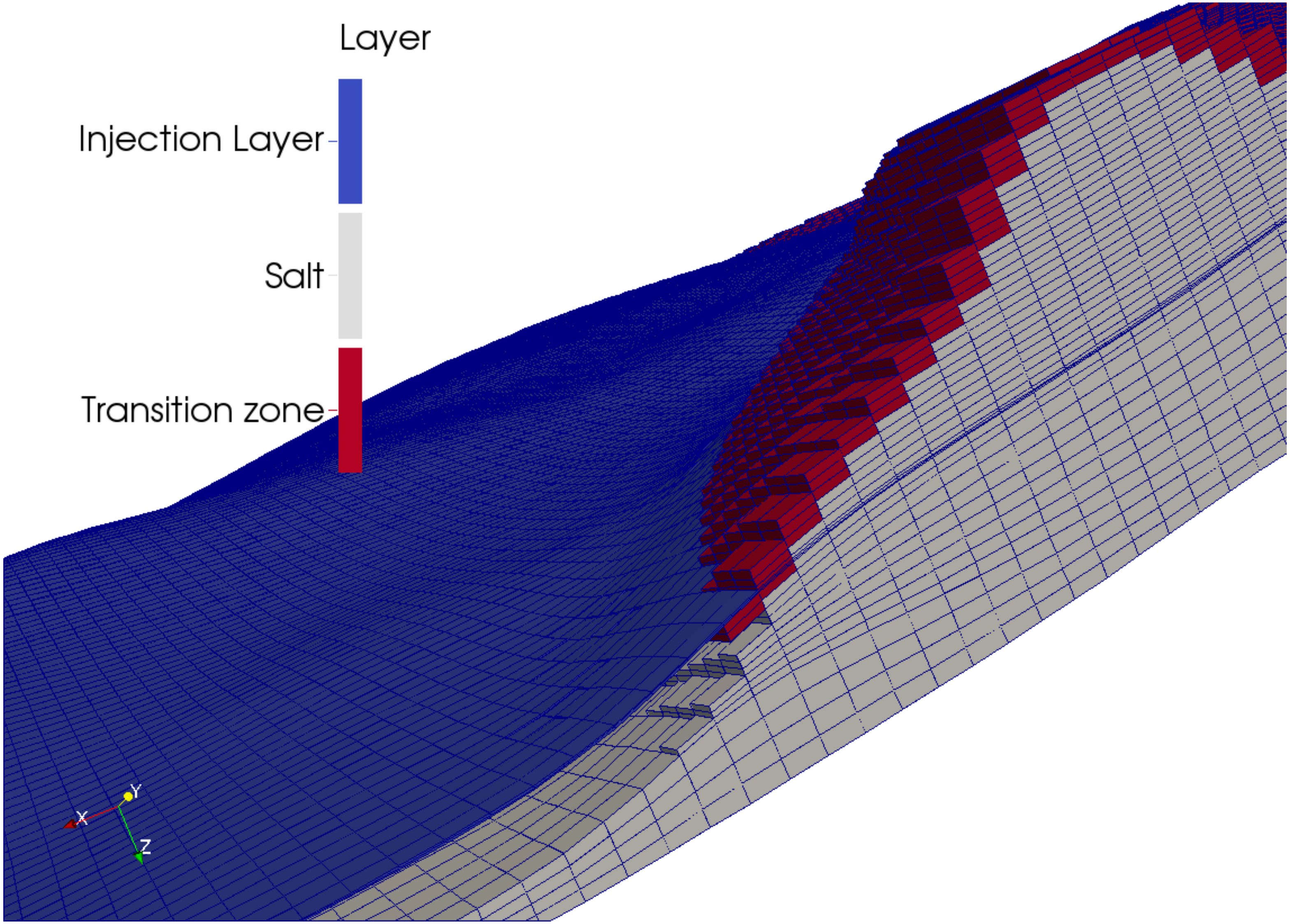
Salt wall with transition zone (fault zone)



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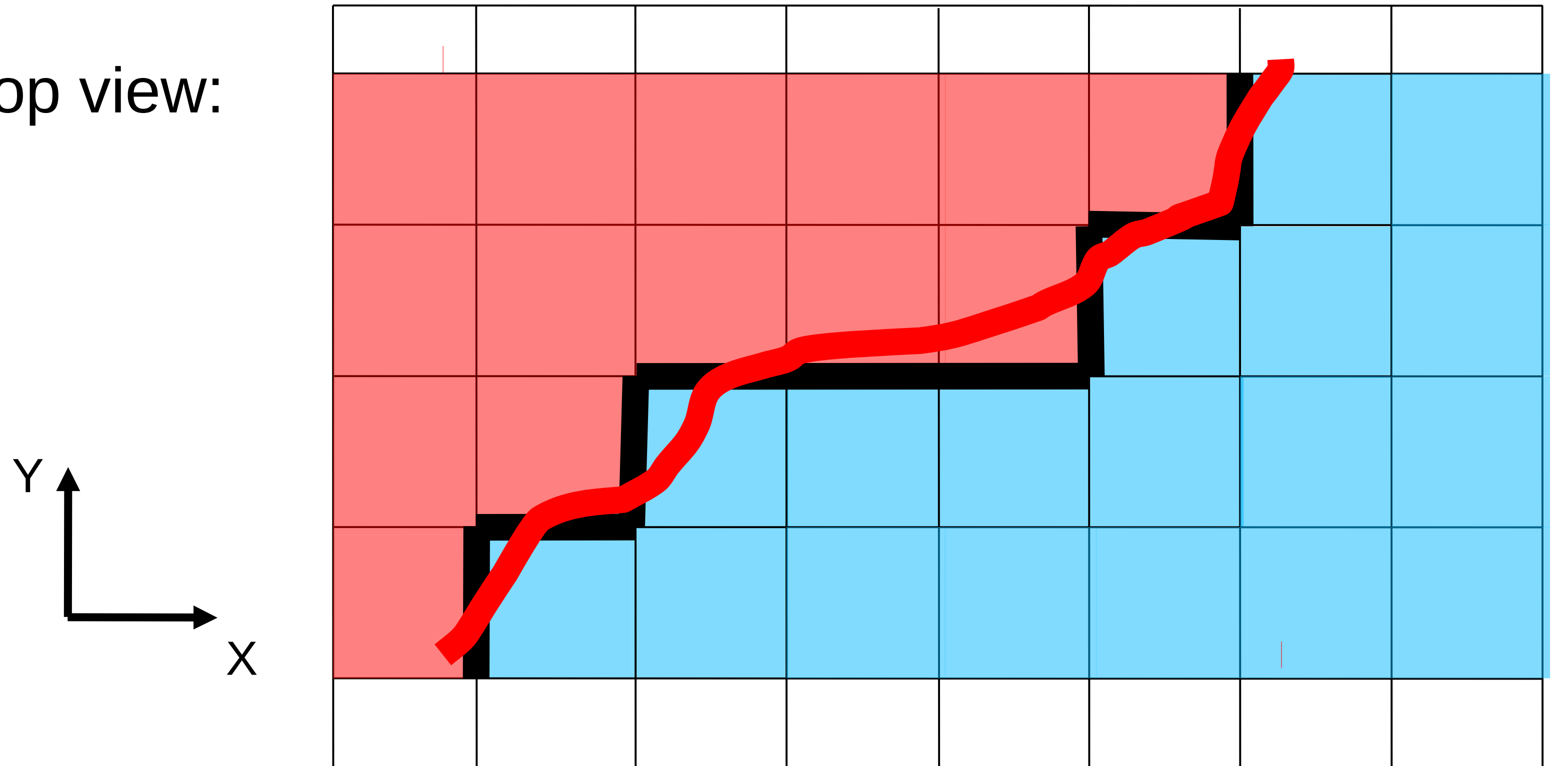
3d Discrete Fracture Model for Fault Zone Representation

- Consider a fault zone embedded in a hexahedron grid
- Fracture lives on the element faces
- Fracture properties are assigned to the element faces

Top view:



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Discrete Fracture Model

- Fracture DOF consider flow in fracture (advective) and matrix (advective + diffusive)

  Total Flow = Fracture Flow + Matrix Flow

  - Two point flux approximation between two fracture DOF for fracture flow

  - Additional parameters *fracture width*, *fracture porosity* and *fracture permeability*.

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Discrete Fracture Model

- Advantages
  - Easy to implement with any kind of grid (Hexahedron, Tetrahedron, Prism etc.)
  - No additional DOF
  - Fracture transmissivity is preserved
- Disadvantages
  - In our case (not refined around the fracture) it is a crude approximation of the geometry
  - For component transport: Additional assumptions on fracture – matrix exchange have to be made

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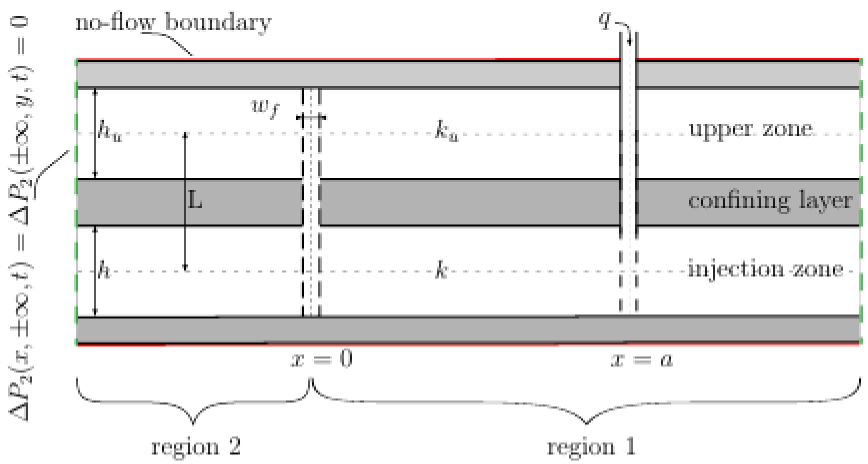
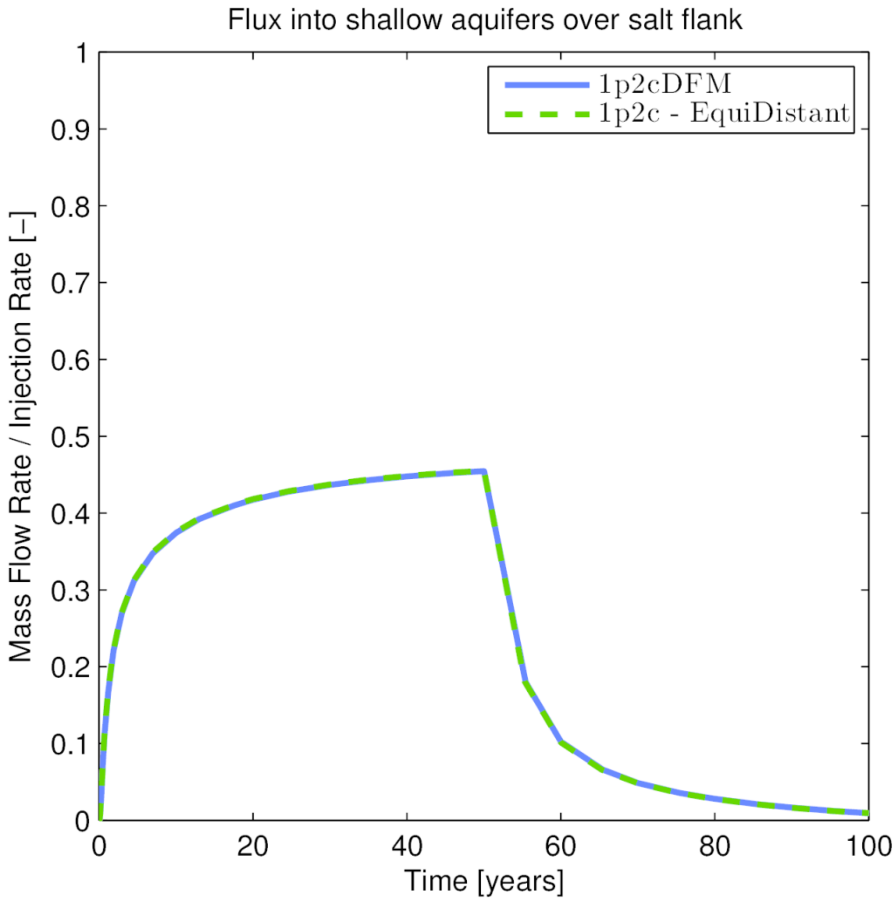
Comparison to equi-distant solution for simple two layer geometry and single phase, single component flow





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DFM implementation in Dumux

- A general DFM model (2d and 3d) has been implemented for the box method
- The general model takes care of the fracture geometry
- Implicit models can be used on top of that like 1p2cdfm and 2pdfm with some model specific adjustments (fracture – matrix exchange etc.)
- No non-isothermal fracture model as yet
- Fracture faces and properties are assigned in the Spatial Parameters

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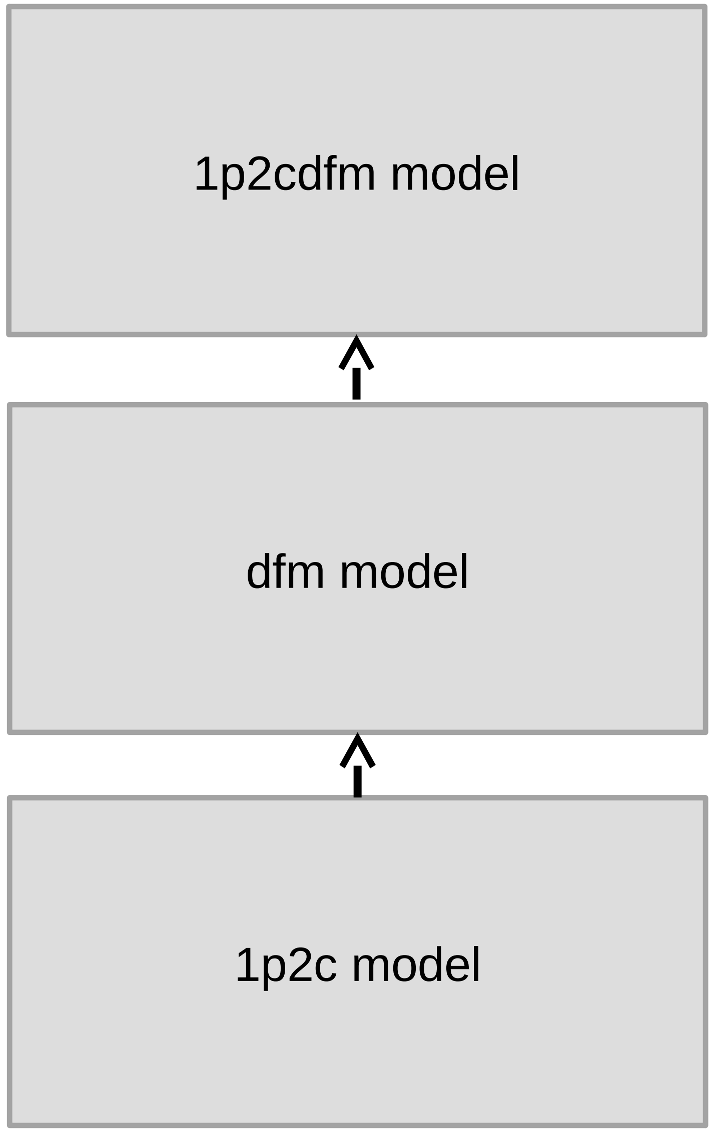
Structure DFM model



Calibration: iTough2 and Dumux

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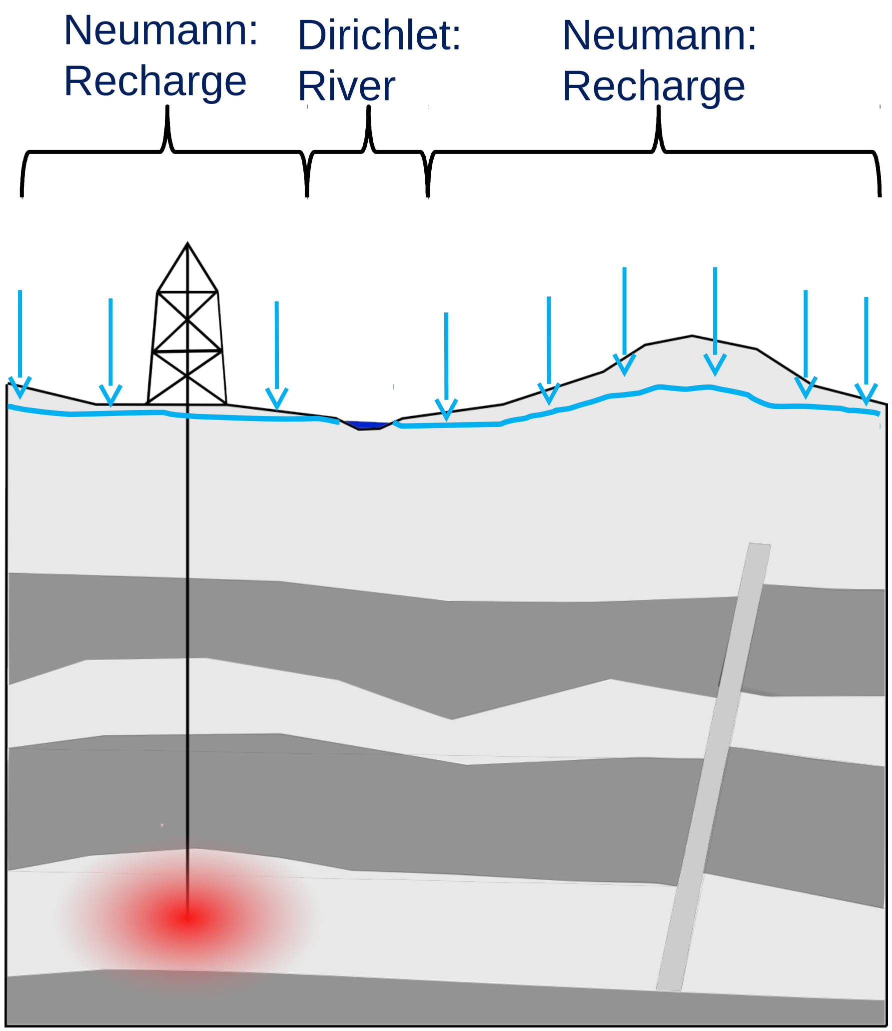
Stationary calibration to obtain natural flow conditions



Possible optimization parameters:

- Top Aquifer permeability
- Recharge rate

Observation points:

- Choose points from groundwater table

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Workflow iTough2 - Dumux

- You require iTough2 using the PEST protocol in order to run iTough2 with other software than Tough2
- Adjust your Dumux problem:
  - Optimization parameters must be specified through the Dumux input file, so that they can be changed by iTough2
  - Write a data file for the observation points which can be written for example in postTimeStep() function in your problem or at the end of your simulation
- Setup the iTough2 input file with your parameters and observation data for more information please refer to *Finsterle (2010)*
- During an iTough2 run Dumux will be started repeatedly with different parameters for the forward runs and for setting up the Jacobian Matrix
- Important turning screws are of course the optimization parameters but also the weighting you assign for your observation points (standard deviation)

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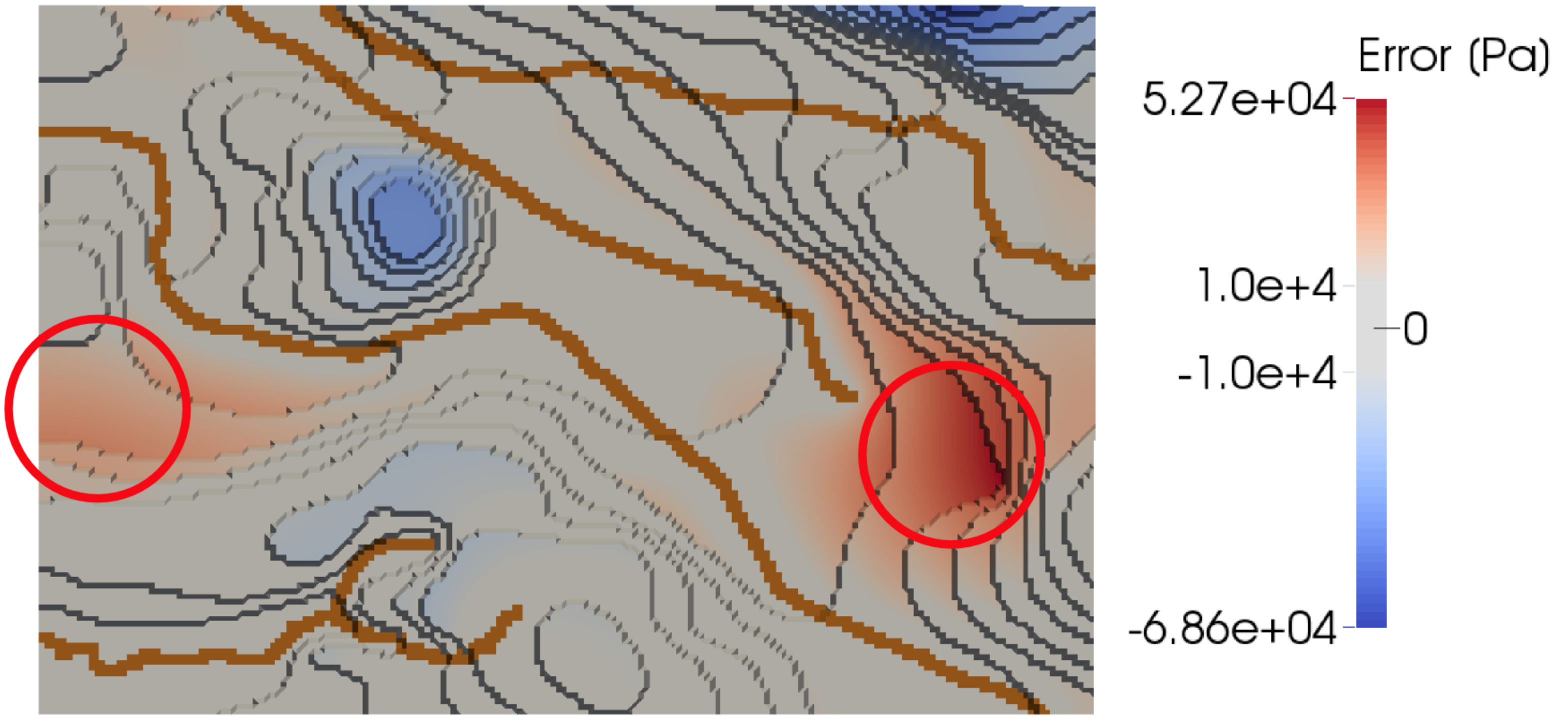
Results: Top view groundwater table

- Only one parameter varied: Perameability of top layer
- Reduced the weight of observation points in the two areas with the red circle. Observations are not trusted here



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Software and Guides

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- Finsterle, S., iTOUGH2 Universal Optimization Using the PEST Protocol, Report LBNL-LB3698E, Lawrence Berkeley National Laboratory, Berkeley, Calif., July 2010.
- Finsterle, S., iTOUGH2 User's Guide, Report LBNL-40040, Lawrence Berkeley National Laboratory, Berkeley, Calif., February 2007.
- Becker, B., Beck, M., Fetzer, T., Flemisch, B., Grüninger, C., Hommel, J., Jambhekar, V., Kissinger, A., Koch, T., Schneider, M., Schröder, N. and N. Schwenck (2015): DuMuX 2.7.0. doi:10.5281/zenodo.16722.