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Supplement of

AREHS: effects of changing boundary conditions on the development of hydrogeological systems: numerical long-term modelling considering thermal–hydraulic–mechanical(–chemical) coupled effects

René Kahnt et al.

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AREHS:
Effects of changing boundary conditions on the evolution of hydrogeological systems: Numerical long-term modeling considering thermal-hydraulic-mechanical (-chemical) coupled effects (Ref-ID: 4719F10402)

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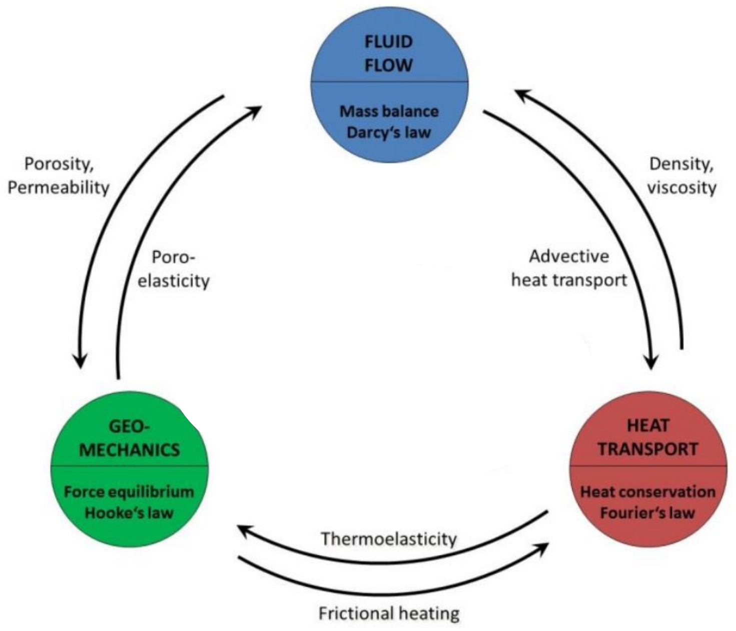
ID: FKZ 4719F10402

The presentation reflects the opinion of the AREAS research team but does not necessarily represent the opinion of BASE

Objectives of AREHS

- Future cold and warm periods and associated glaciation events will change the (petro-) physical properties as well as the natural hydrogeological properties of the overall system and especially in the host rock
- This has to be well understood quantitatively to be able to conduct long term safety analysis
- The objective of AREHS is the development of a THM(C) -modeling toolbox to simulate the impacts of the changing boundary conditions on all three types of host rocks (salt, clay and crystalline rocks)
- To increase the confidence in the numerical codes, this modeling toolbox has to be verified



From Gaucher u. a., 2015

Structure of the research project

WP 1: Literature survey:

- Compilation of input data and development of a data base,
- Climate models for 1 mill. yrs
- Geological conditions in Germany
- State of the art of coupled THM(C)-modelling in geoscience

WP 2: Development of a THM-(C) model approach:

- Physical characterization of the problem
- Mathematical equations incl. coupling
- Analytical solutions and 1D-THM-(C)-models for all three host rocks
- Benchmark published field data on THM (C) processes from at least one case study of a large-scale geoscience application three host rocks
- Benchmark for reproducing field data on past icing events three host rocks
- Benchmark with published modelling results three host rocks

WP 3: Modeling the effects of future icing cycles on THM-(C) processes

- Definition of the model area and creation of the 3D geological models as a basis for the dynamic simulations
- Formulation of the initial and boundary conditions incl. modelling approach
- THM-(C) – modelling for clay rock
- THM-(C) – modelling for salt rock
- THM-(C) – modelling for crystalline rock
- Comparison of the model approaches and the results

WP 4: Report

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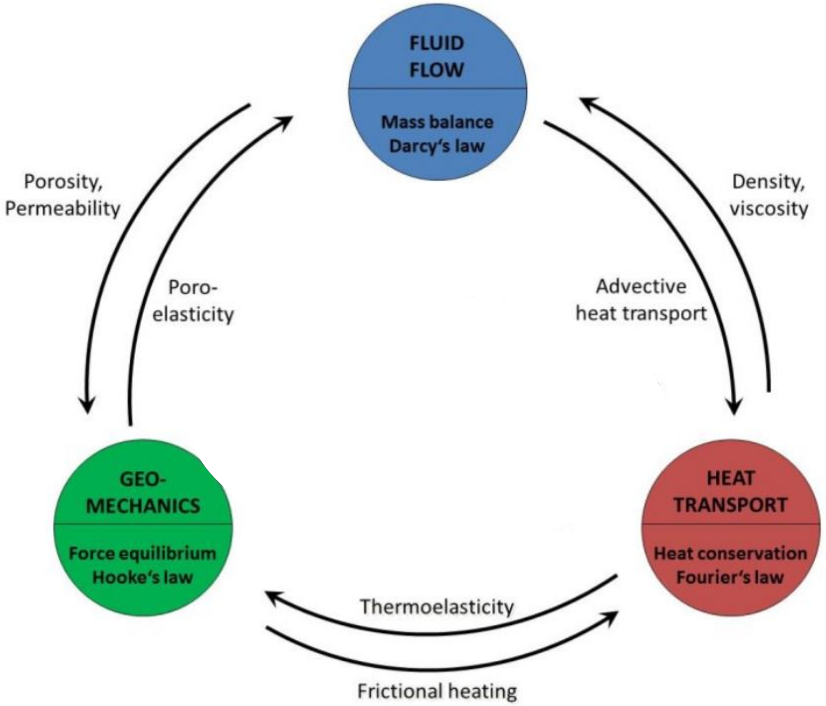
WP 4: Report

Processes and numerical codes

Basic processes and coupling:



From Gaucher u. a., 2015

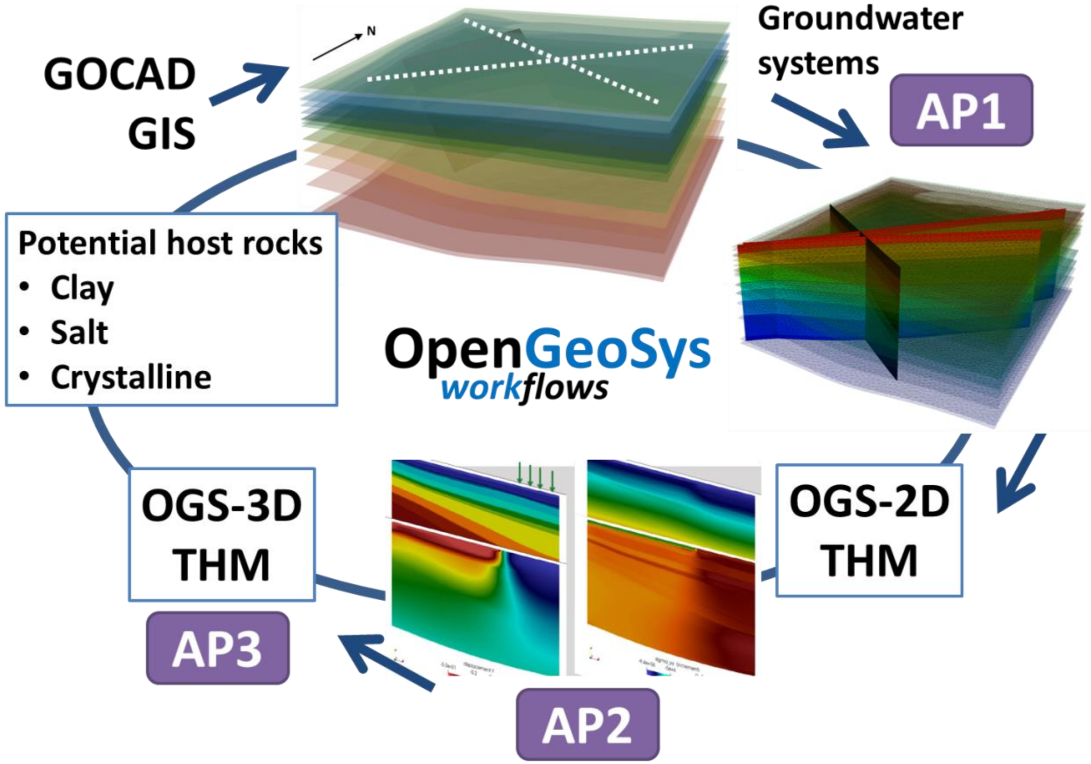
Numerical codes:

Salt rock:	OpenGeoSys
Clay rock:	OpenGeoSys
Crystalline rock:	3DEC + DFN.lab

WP 2: Example 1

Benchmark for reproducing field data on past icing events and benchmark with published modelling results for salt rock

Workflow implementation OGS



- Development of a workflow for 2D vertical sections and 3D OGS models from GOCAD/GIS projects
- Automation of the workflow concept with container technologies (contains all data/code for the complete application)
- Simulation of cold-warm times (glaciation)

AP2: Salt dome – Halokinesis: Model setup

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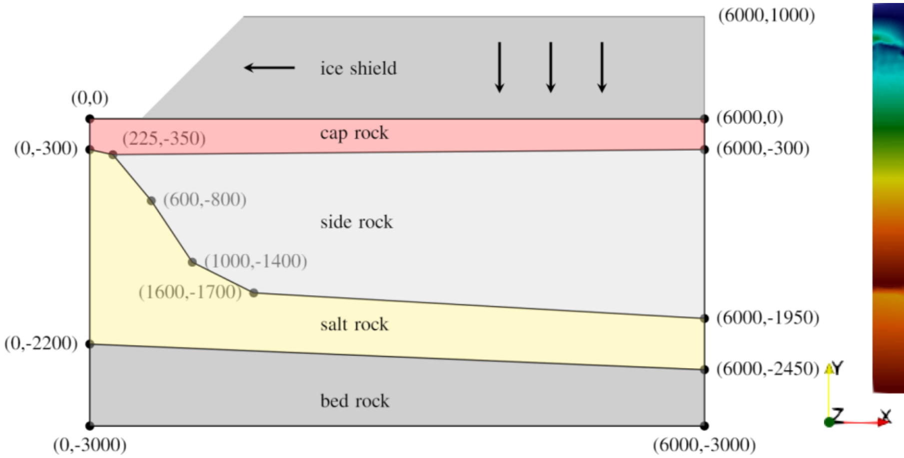
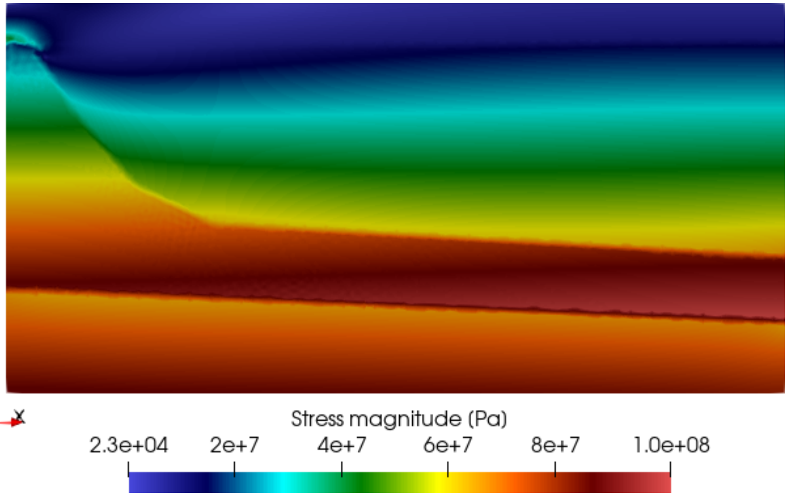
Comparison with simulations from literature – OGS-Simulation

- Model description according to Bruns et al. (2012).
- Loading of model under self-weight for 1 million years equilibrium state for plastic creeping in salt.
- Result provides initial stress state for glacier crossing



Model geometry (glacier als load boundary conditions)



Stress magnitude after 1 mill. yr. (THM coupling)

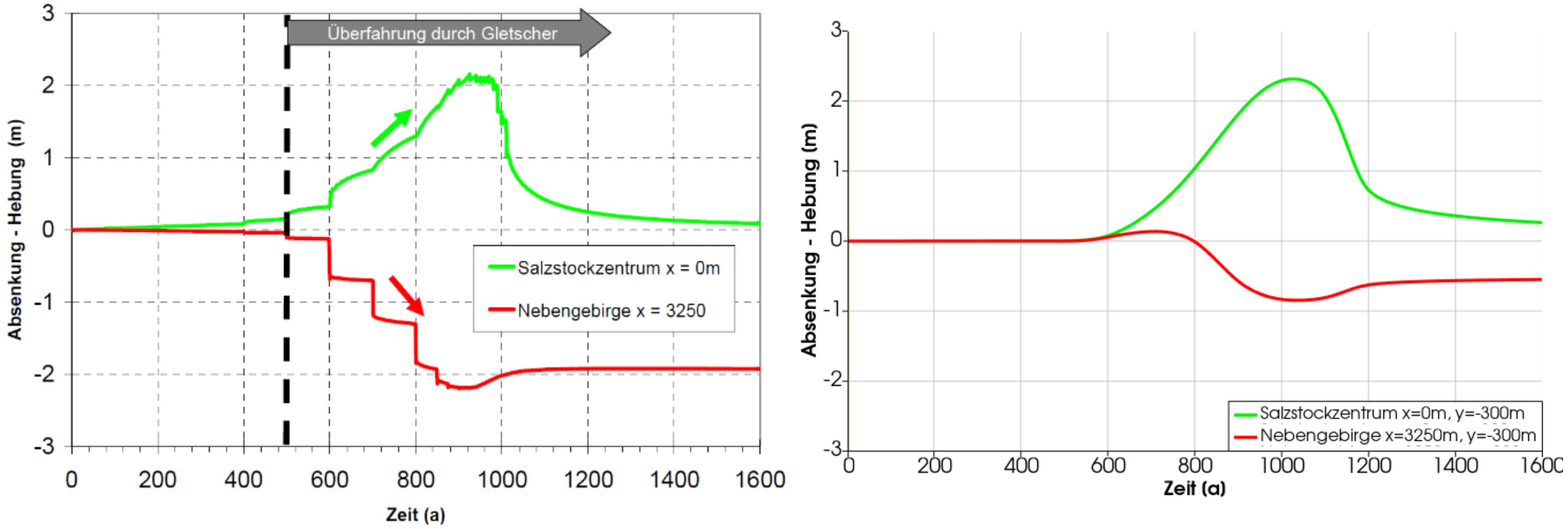
Bruns, J, L Boetticher, H Doose, M Cottrell, P Wolff, R.-M. Günther, D Naumann, T Popp und K Salzer (Aug. 2012).Glazigene Beeinflussung von Wirtsgesteinstypen Ton und Salz und deren Einflüsse auf die Eignung zur Aufnahme eines HAW-Endlagers.Techn. Ber. Celle: Golder Associates GmbH in Kooperation mit IfG Institut für Gebirgsmechanik GmbH, S. 292

AP2: Salt dome – Halokinesis: Results

AP2: Salt dome – glacier propagation

Comparison Bruns – OGS-Simulation

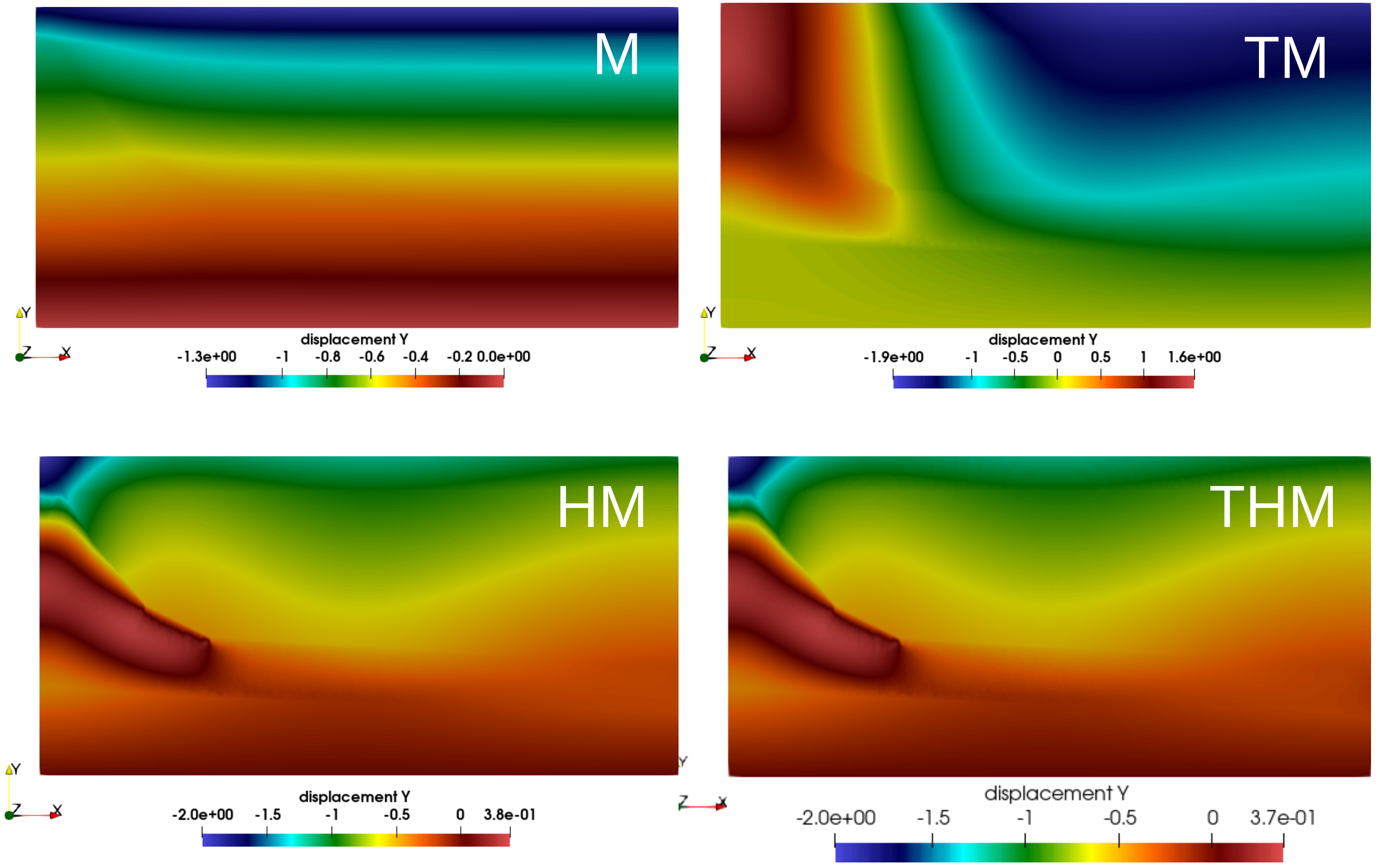
- Glacier crossing results in uplift of salt dome and subsidence of side rock
- Qualitatively similar results
- The subsidence modelled in OGS is smaller than modelled by Bruns (different material model, Bruns uses interface elements between salt and hanging wall, OGS without)



Comparison of the vertical displacement at two measurement points during a glacier crossing between the study (left, Bruns et al.,2012) and the OGS simulation (right).

AP2: Salt dome – Halokinesis: Process coupling

- Investigation of the influence of the couplings of the T, H and M processes on the model behavior.
- Hydraulics seem to have a greater influence than thermal coupling
- Mechanics alone are not sufficient to simulate the system adequately - process coupling has a clear influence



- Vertical displacement after complete glacier propagation cycle

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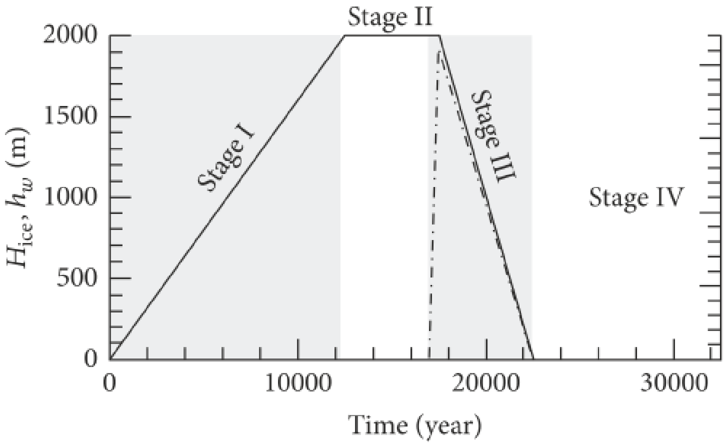
WP 2: Example 2

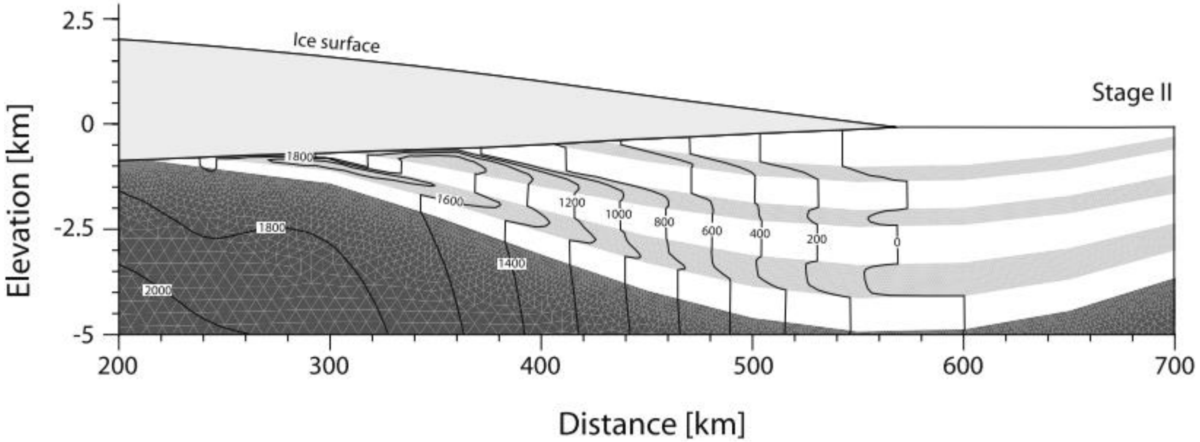
Benchmark for reproducing field data on past icing events and benchmark with published modelling results for clay rock

Benchmark for reproducing field data on past icing events and Benchmark with published modelling results for clay rock

Icing events/cycles



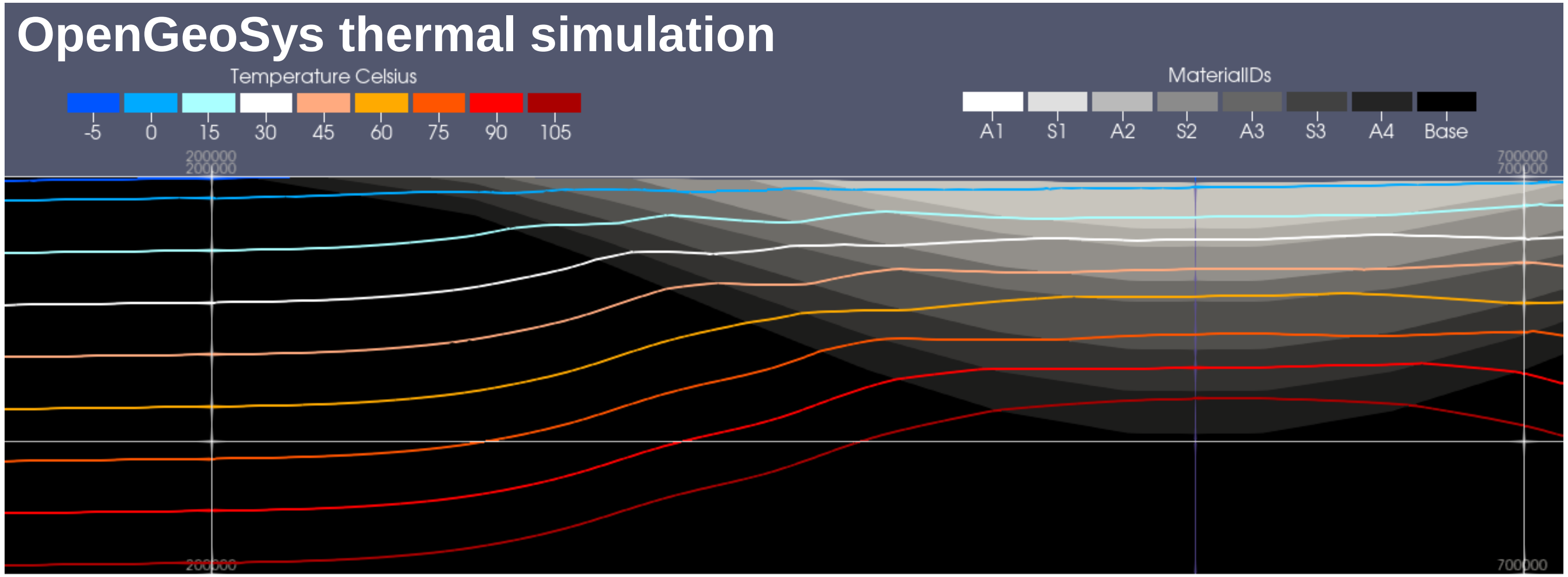
Glacier height evolution from *Bense and Person, 2008; Bea et al., 2018*



Sedimentary basin with glacier advance from *Bense and Person, 2008; Bea et al., 2018*

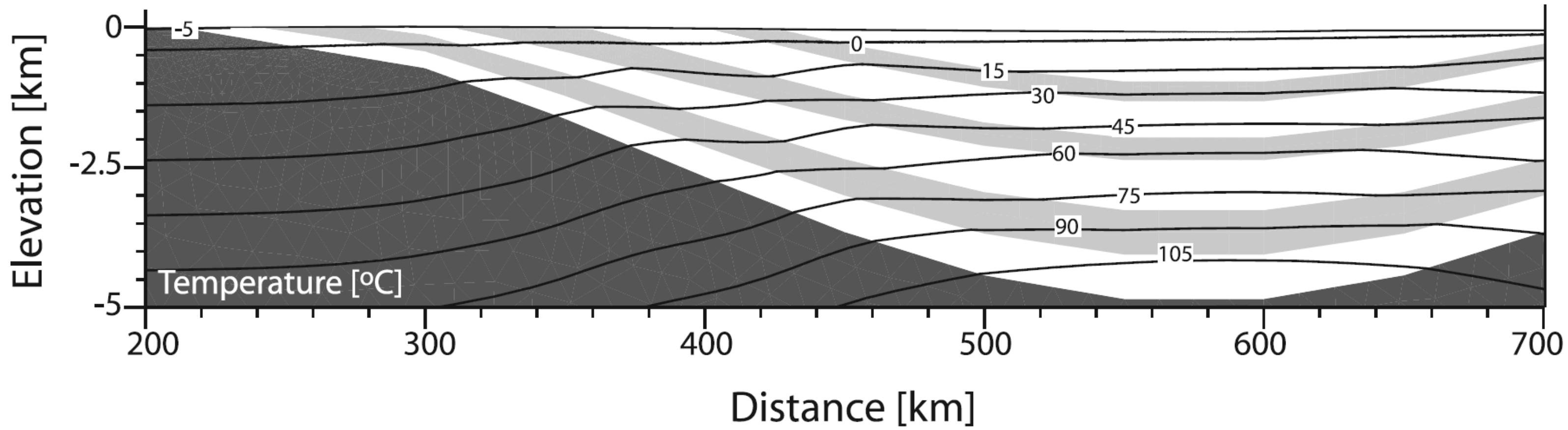
- Glaciers captured by transient BCs (load, temperature, hydraulic head)
- Consideration of freezing and thawing processes incl. development of the ground frost body
- Permafrost: several couplings (TH, TM), for example: temperature dependent soil properties, reduction of ground water flow and changed thermal gradients, …

Benchmark for reproducing field data on past icing events and Benchmark with published modelling results for clay rock



OpenGeoSys, thermal simulation:

Initial state



Corresponding result from Bense and Person, 2008

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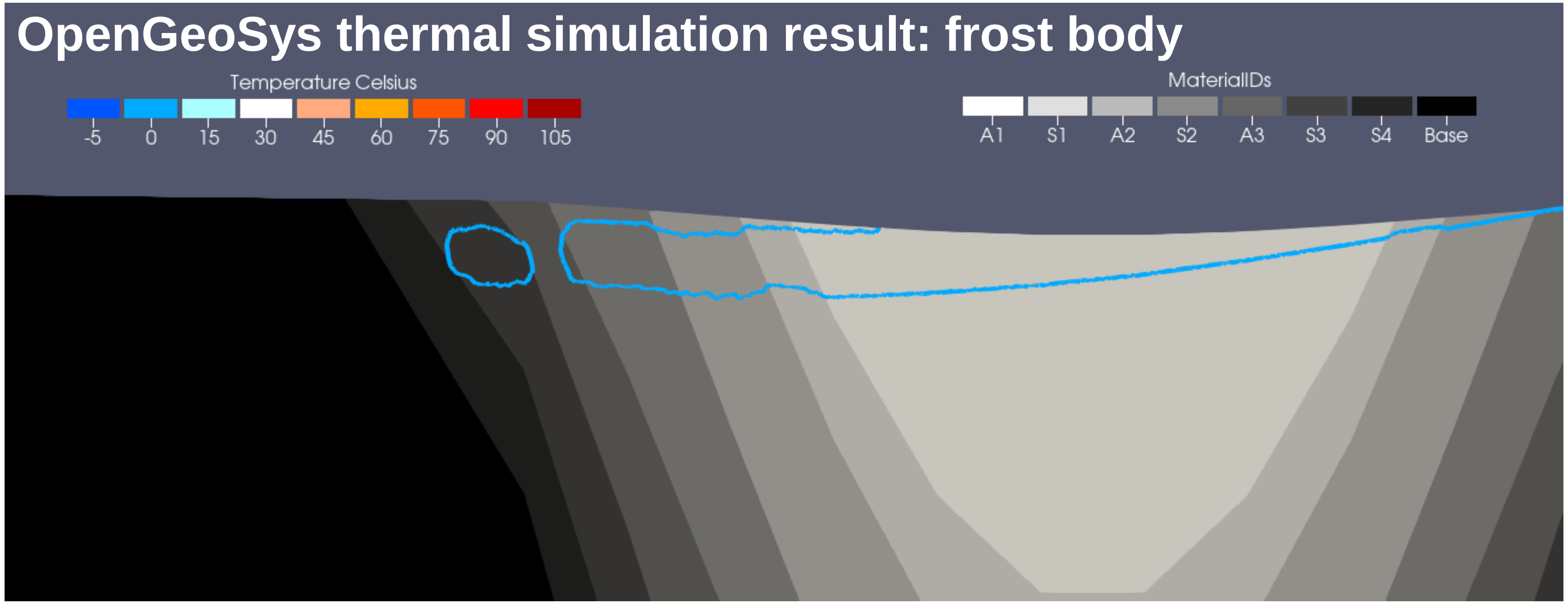
Benchmark for reproducing field data on past icing events and Benchmark with published modelling results for clay rock



Frost body evolution during glacier advance (vertical exaggeration 10)

- blue polygons show frozen regions
- delayed thawing in the sediment layers: emergence of ice lense

Benchmark for reproducing field data on past icing events and Benchmark with published modelling results for clay rock

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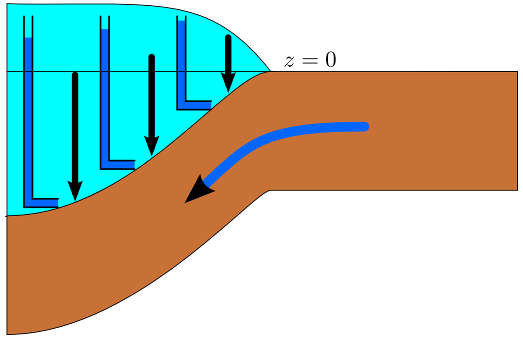
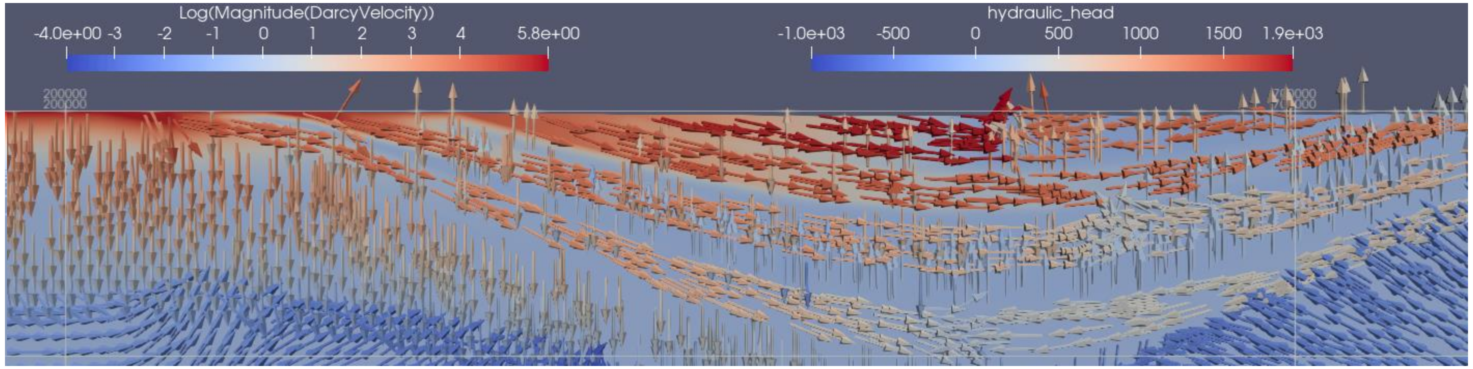
OpenGeoSys hydraulic - (mechanical) simulation for clay rock

Example scenarios for plausibility check:



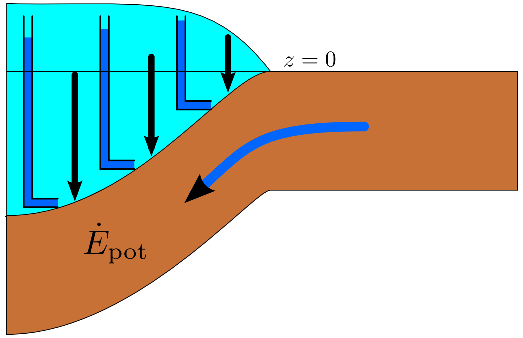


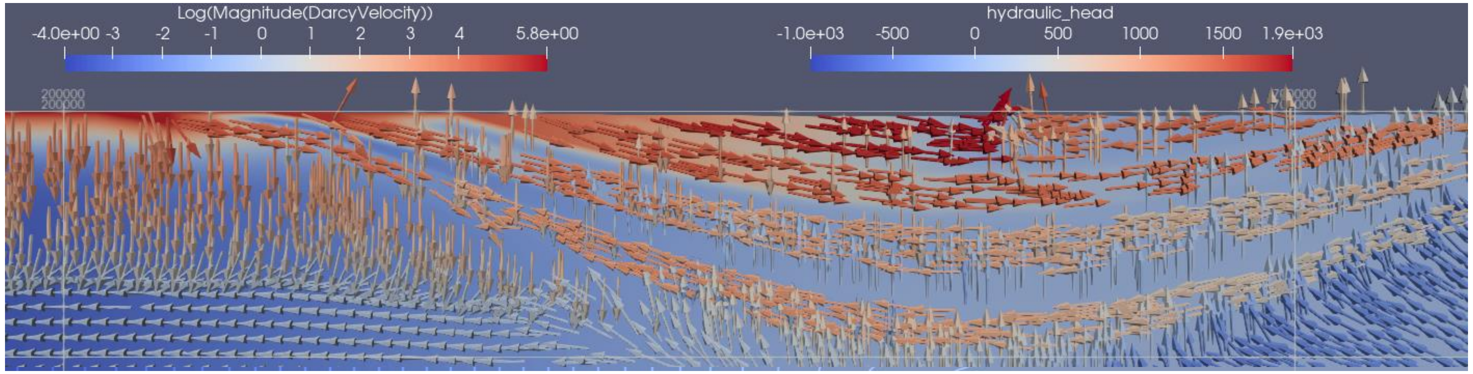
h-BC at the top:

Glacier pressure and vertical movement of the lithosphere

h-source term:

/





h-BC at the top:

Glacier pressure and vertical movement of the lithosphere

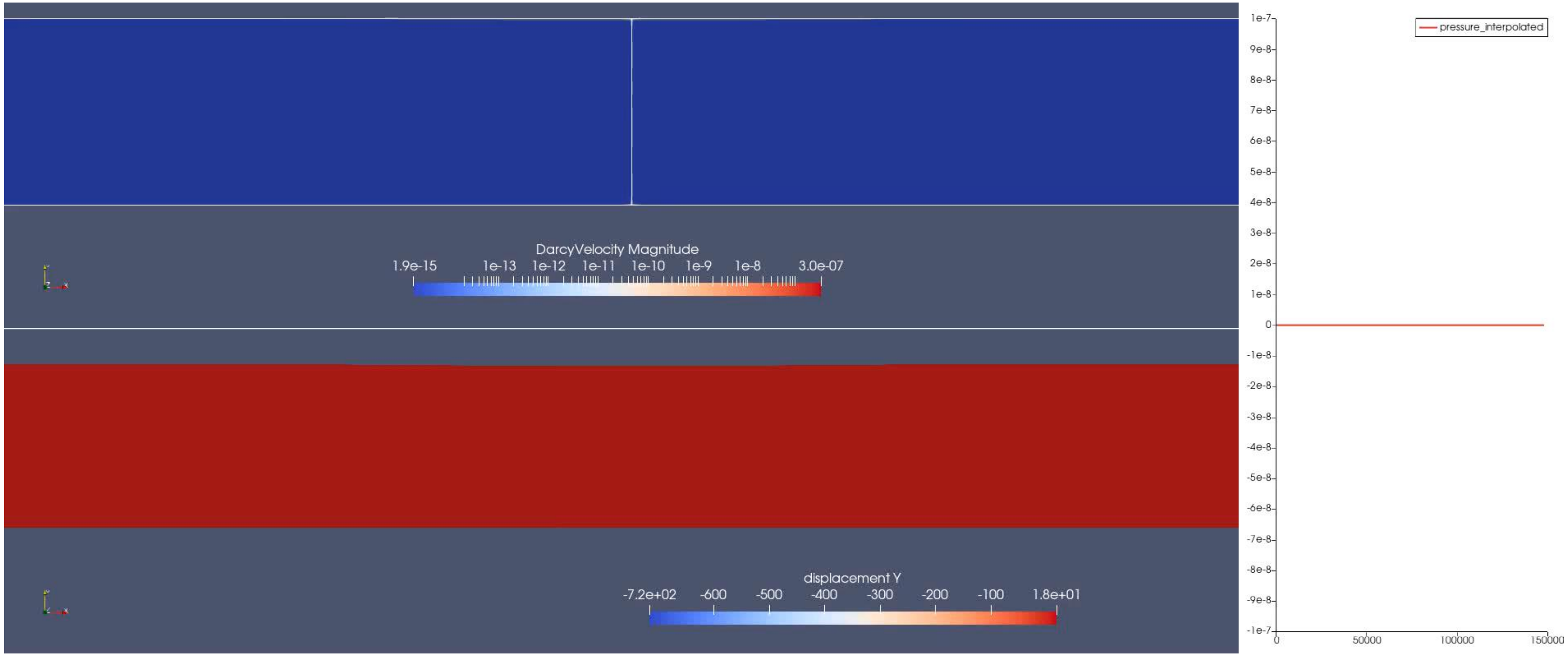
h-source term:

rate of vertical movement of the lithosphere

AP 2.5 & AP 2.6: Benchmark zur Reproduktion von Felddaten zu vergangenen Vereisungsereignissen / Benchmark mit veröffentlichten Modellierungsergebnissen

OpenGeoSys fully coupled hydraulic - mechanical simulation for clay rock

Pilot simulation results considering the deformation under the glacial load



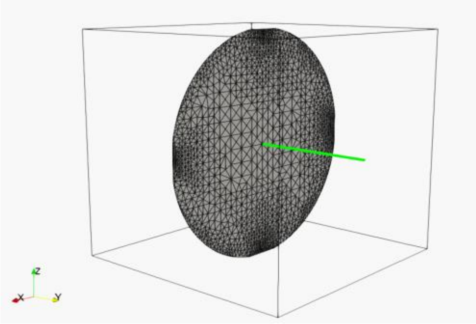
WP 2: Example 3

Benchmark with analytical solutions for crystalline rock and model coupling concept 3DEC-DFN.Lab

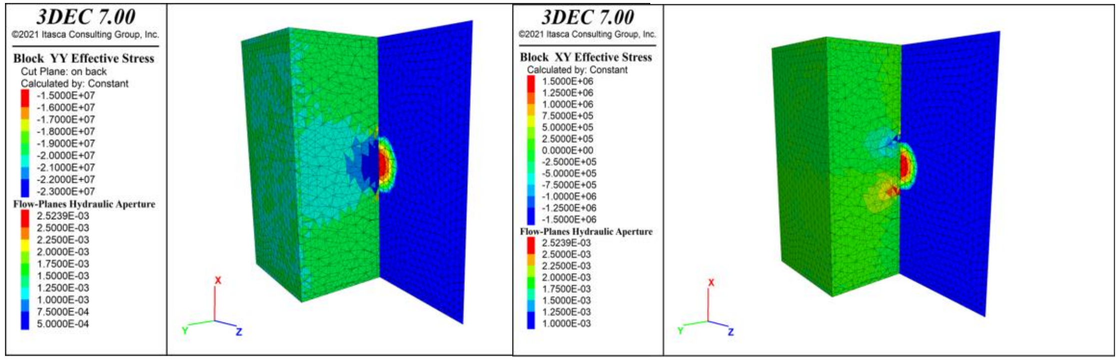
AP2: Fracture opening in crystalline rock

Model Description:

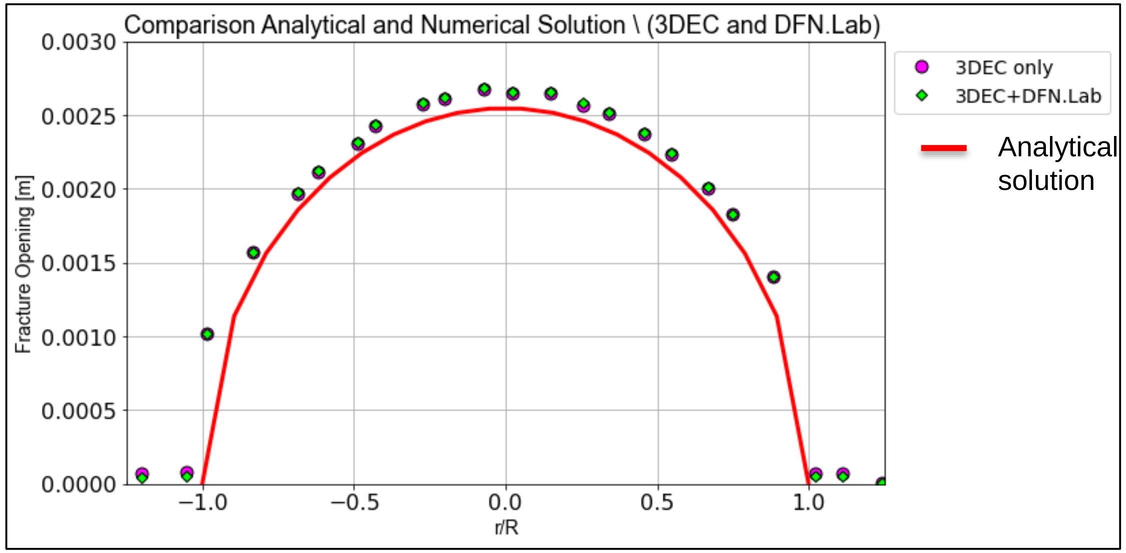
1. Injection into single fracture (DFN.Lab Calculation)
2. Import of the hydraulic pressure field into 3DEC – block model
3. Calculating fracture opening/mechanical response due to increased hydraulic pressure (3DEC Calculation)



DFN.Lab model of the single fracture with indication of the injection location



Calculated stress field in 3DEC block model after pressure import



Comparison of the fracture opening calculated in 3DEC and 3DEC+DFN.Lab with the analytical solution of (Sneddon, 1946; Green and Sneddon, 1950)

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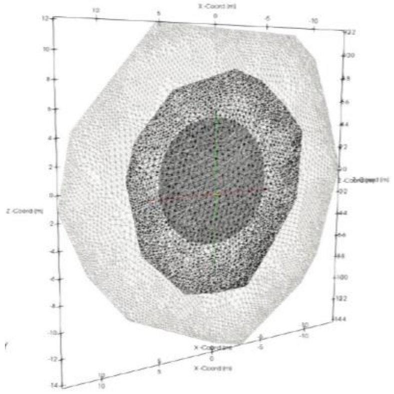
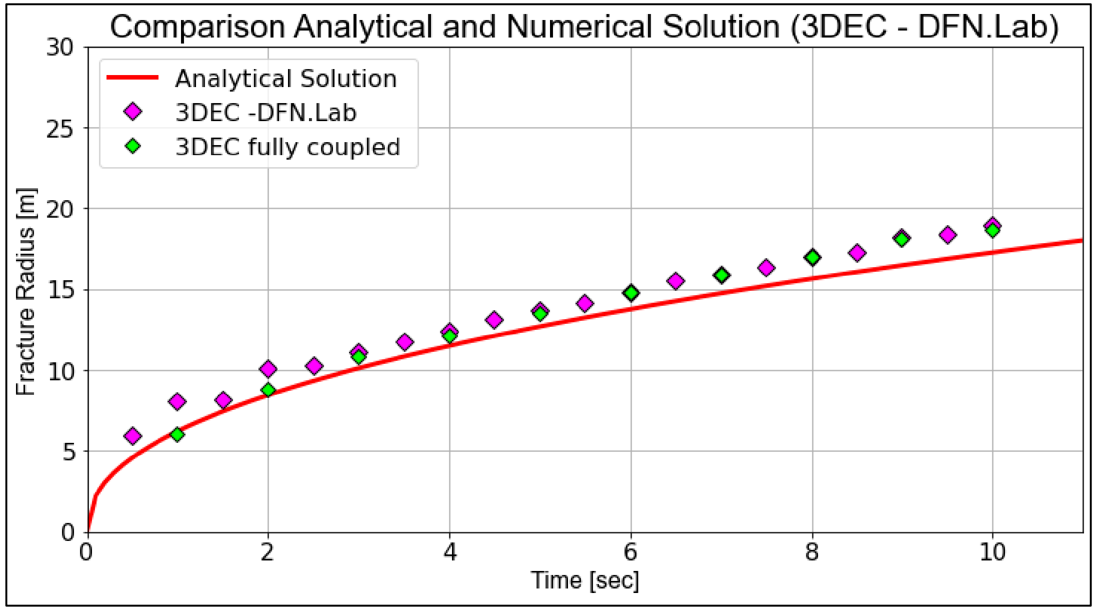
AP2: Fracture opening in crystalline rock

Model Description:

1. Injection P(t) into single fracture (DFN.Lab Calculation)
2. Import of the hydraulic pressure field into 3DEC – block model
3. Calculating fracture opening and growth due to increased hydraulic pressure (3DEC Calculation)
4. Update fracture contour
5. Injection P(t+1) into updated fracture

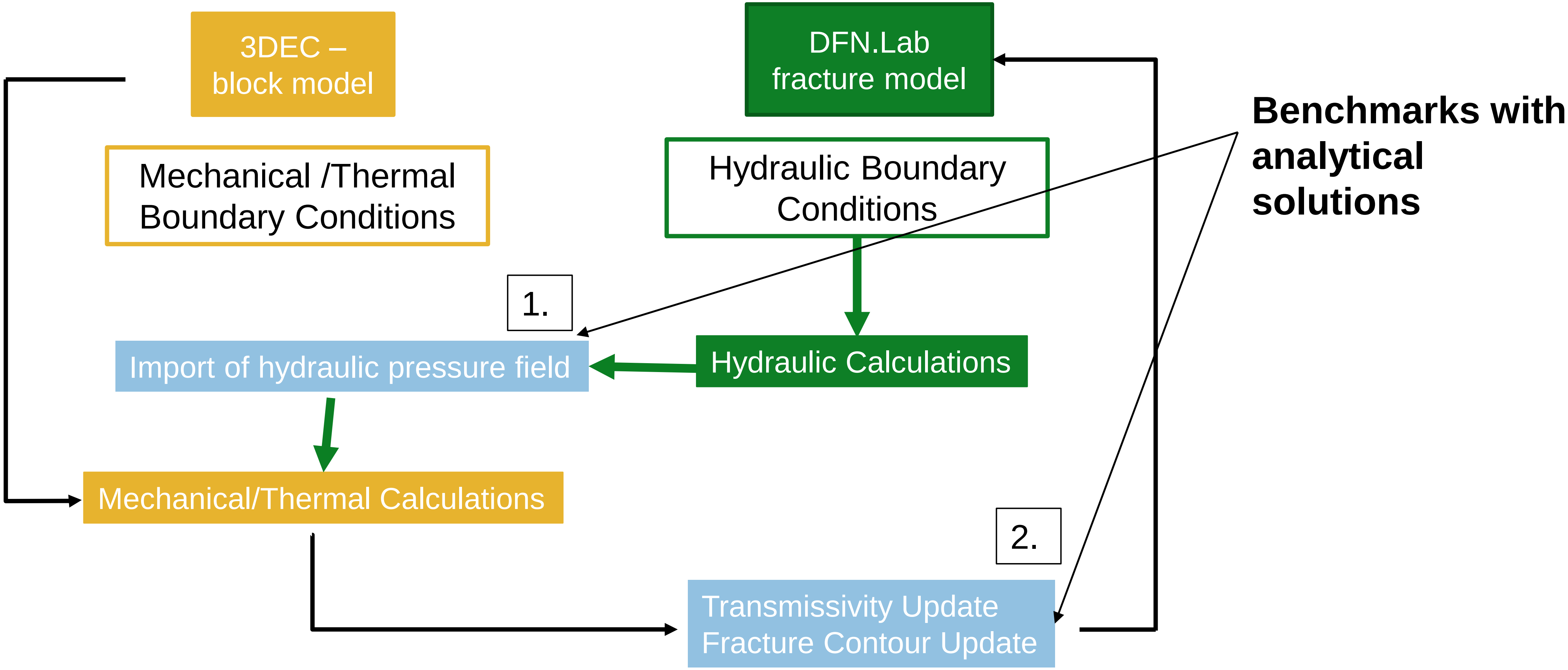


DFN.Lab model of the single fracture. There are 3 different fracture contours indicated. The fracture contour is determined by the convex hull of the failed subcontacts in 3DEC

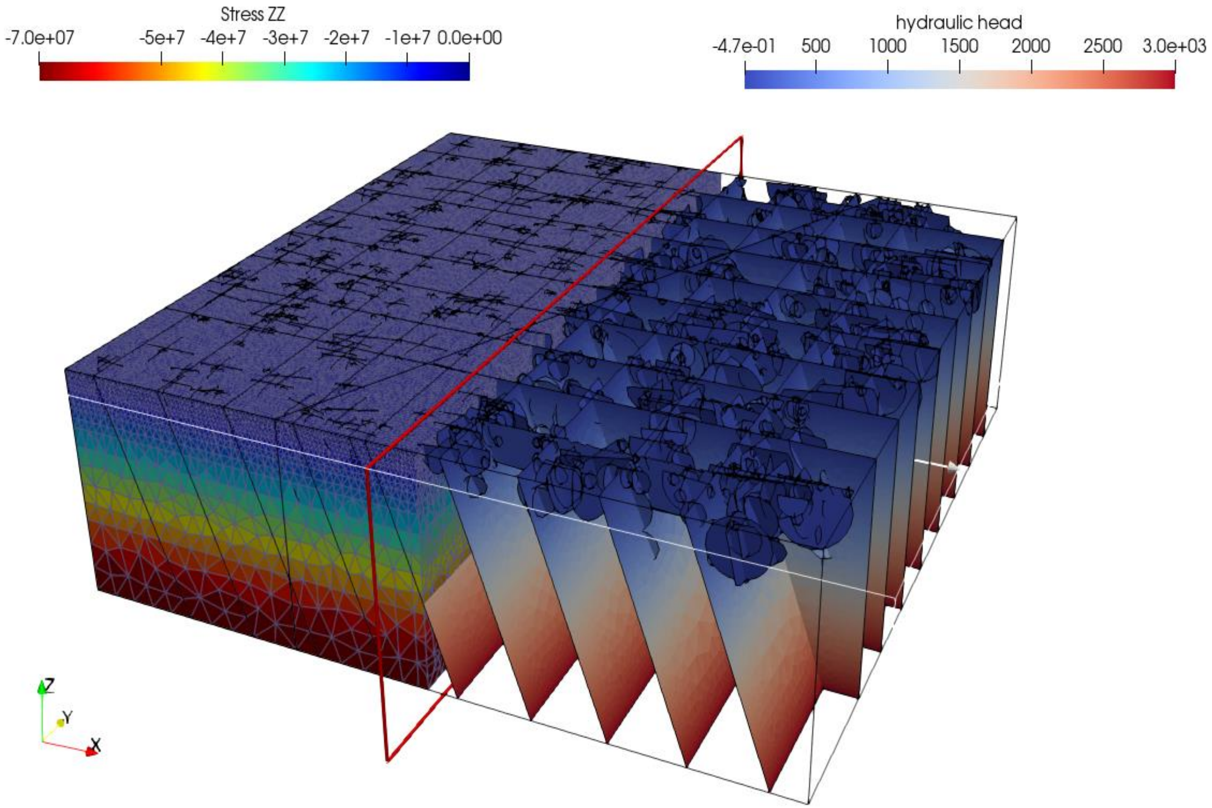


Comparison of the fracture growth calculated in 3DEC and 3DEC+DFN.Lab with the analytical solution of (Perkins and Kern, 1961; Geertsma and De Klerk, 1969)

AP2: Fracture opening in crystalline rock



AP2: Fracture opening in crystalline rock



Generic model of the crystalline host rock (left: 3EDC, right: DFN-lab) including DFN of different scales indication the mechanical and hydraulic pressure field

Considering discontinuities of different scales by incorporating a complex „Discrete Fracture Network“ (faults and fractures)

→ Performing thermo-mechanical calculations with the DEM-Software “3DEC“ (Itasca, 2020)

→ Performing hydraulic calculations with the DFN-Software “DFN.Lab“ (Le Goc et al., 2020) *(Assumption: matrix flow in comparison to joint flow negligible)*

AP3: Selection of processes based on FEP catalogues

AP3: Selection of processes based on FEP catalogues

Selection of relevant FEPs:

1. External Factors
- 1.1 Repository Issues (pre-closure)
- 1.2 Geological Factors
- 1.3 Climatic Factors
- 1.4 Future Human Actions
- 1.5 Other External Factors

2. Waste Package Factors
- 2.1 Waste Form
- 2.2 Waste Packaging Characteristics and Properties
- 2.3 Waste Package Processes
- 2.4 Contaminant Release [waste form]
- 2.5 Contaminant Migration [waste package]

3. Repository Factors
- 3.1 Repository Characteristics and Properties
- 3.2 Repository Processes
- 3.3 Contaminant Migration [repository]

4. Geosphere Factors
- 4.1 Geosphere Characteristics and Properties
- 4.2 Geosphere Processes
- 4.3 Contaminant Migration [geosphere]

5. Biosphere Factors
- 5.1 Surface Environment
- 5.2 Human Characteristics and Behavior
- 5.3 Contaminant Migration [biosphere]
- 5.4 Exposure Factors

FEP-Table of Energy Agency: NEA FEP Database https://www.oecd-nea.org/fepdb/login/

AP3: Selection of processes based on FEP catalogues (example)

NEA-Nr. & FEP	Description	Salt	Clay	Crystalline
1. External Factors				
1.3 Climatic Factors				
1.3.1 “Global Climate Change”	Global climatic change	Climate episodes	Climate episodes	Climate episodes
1.3.4 “Periglacial Effects”	Periglacial Effects (Frozing and melting)	BC (T) Phase transition	BC (T) Phase transition	BC (T) Phase transition
1.3.5 “Glacial and ice-Sheet Effects”	Inland icing – glacier load	BC (M)	BC (M)	BC (M)
	Inland icing – „warm-glacier base“ Increased reacharge	BC (H)	BC (H)	BC (H)
	Thermal insulation by glacier Gletscher	BC (T)	BC (T)	BC (T)
1.3.7 “Hydrogeo-logical response to climate change”	Hydrogeological response to climate change covered by physical coupling	THM	THM	THM

AP3: Selection of processes based on FEP catalogues

FEPs covered by scenarios

NEA – Nr.	FEP	Description	Salt	Clay	Crystalline
1. External Factors					
1.2 Geological Factors					
1.2.3	„Deformation (elastic, plastic, or brittle)”	Tectonically superimposed external deformation processes	Covered by specific scenarios?	Covered by specific scenarios?	Covered by specific scenarios?
1.2.4	„Seismicity“	Seismicity induced by glacier	Covered by specific scenarios?	Covered by specific scenarios?	Covered by specific scenarios?
1.2.8	„Regional erosion and sedimentation“	Erosion and sedimentation	Covered by specific scenarios	Covered by specific scenarios	-
1.3 Climatic Factors					
1.3.3	“Sea-Level Change”	Transgression and regression	Covered by specific scenarios?	Covered by specific scenarios?	-
1.3.5	“Glacial and ice-Sheet Effects”	Glacial channel formation and erosion caused by glacier	Covered by specific scenarios?	Covered by specific scenarios?	Covered by specific scenarios?

AP3: 3D geological models

Generic models representing typical geological settings

AP 3: Geologcial models salt and clay

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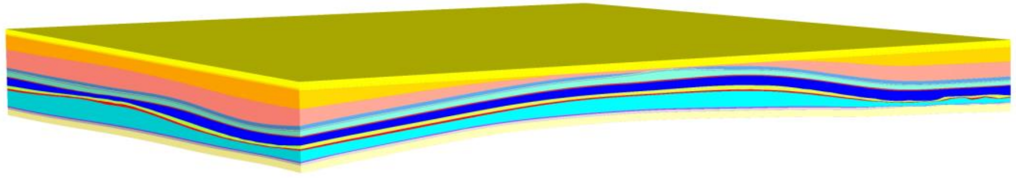
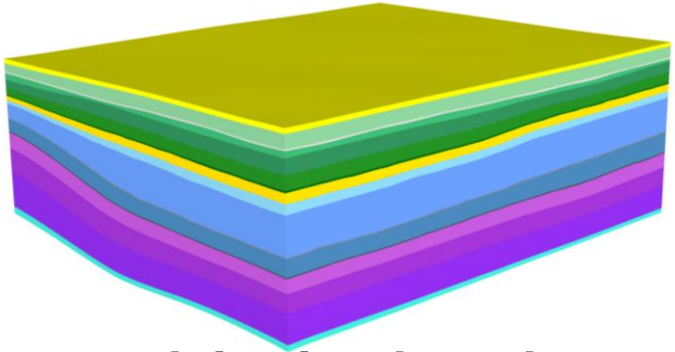
3D-Model: Salt (pillow)

Model area: 12 x 12 km², elevation: 85 m NN to -1400 m NN, Host rock: Staßfurt salt



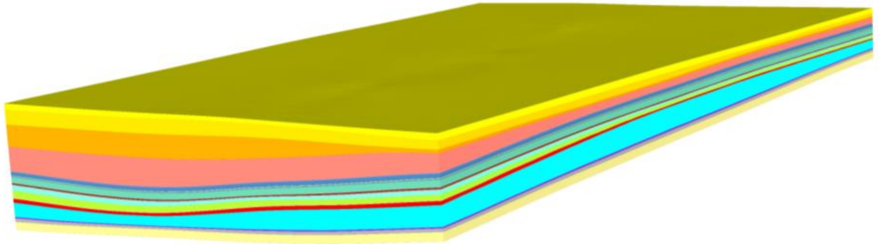
3D-Model: Clay (North Germany)

Model area: 12 x 10 km², elevation 130 m NN to -4200 m NN, Host rock: Barremium and Hauterivium



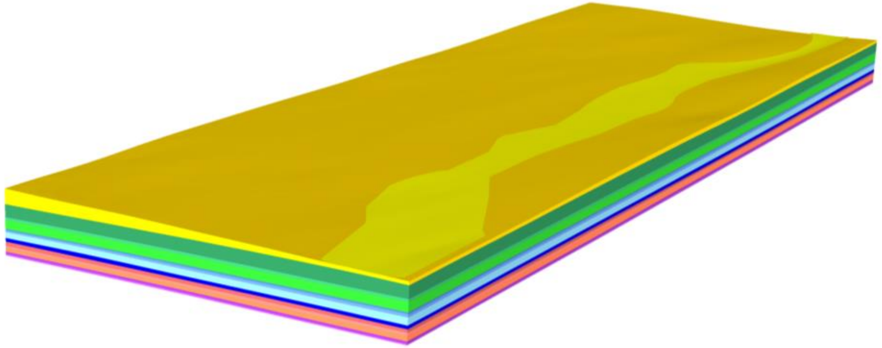
3D-Model: Salt (flat layering)

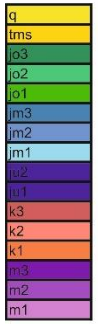
Model area: 10 x 7 km², elevation: 87 m NN to -1500 m NN, Host rock: Staßfurt salt



3D-Model: Clay (South Germany)

Model area: 22 x 7 km², elevation: 565 m NN to -666 m NN, Host rock: Opalinuston





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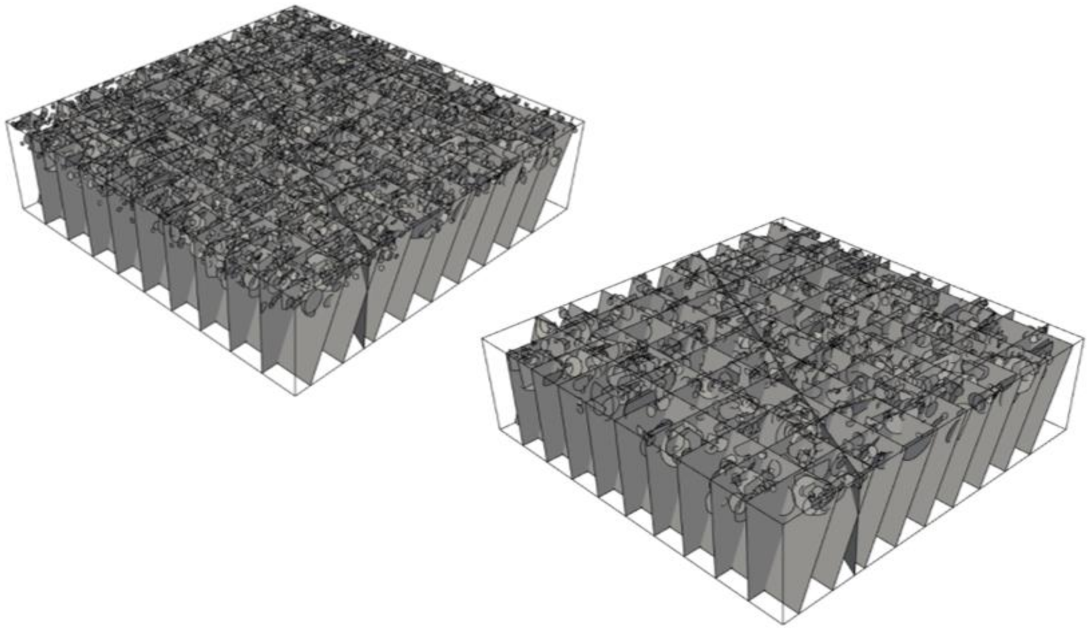
AP 3: Geological model crystalline

AREHS

3D-Model: Crystalline rock – multiple host rock

Assumptions:

- Orthogonal fault network with 1 km distance
- NW-SE striking faults with 70° dips towards NE
- SW-NE striking faults with 90° dips and
- One NNW-SSE striking fault, vertical
- Fracture length > 100 m incorporated in DFN, max. 1000 m
- Fracture density decreases with depths



Regular grid of fault zone (perpenticlular) and arbitrary discrete fracture network; left: original DFN with 5.000 fractures; right: "DFN-Backbone" (filtering of insulated fractures) – hydraulic active DFN.

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Thank you for your attention on behalf of the AREHS team!

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