# Improvement of predictive Quality for Final Repository Site Simulations through Optimal Data Acquisition and <u>Smart</u> <u>Monitoring</u>

### Qian Chen, M.Sc

Prof. Julia Kowalski Dr. Marc S. Boxberg



Chair of Methods for Model-based Development in Computational Engineering Faculty of Mechanical Engineering Nino Menzel, M.Sc

Maria Fernanda Morales, M.Sc

Prof. Florian Wagner



Geophysical Imaging and Monitoring Faculty of Georesources and Materials Engineering apl. Prof. Sergey Oladyshkin Prof. Wolfgang Nowak



Department of Stochastic Simulation and Safety Research for Hydrosystems Institute for Modelling Hydraulic and Environmental Systems Stuttgart Center for Simulation Science

# **Reference model claystone (Northern Germany)**



- Claystones of Barremian and Hauterivian age (cretaceous)
- Depth of host rocks: 500 to 850 m below ground level
- Underlying: Formations of Jurassic and Triassic
- **Overlying**: Upper Cretaceous and **Cenozoic** units
- Model represents geologic conditions of Northern
  Germany (according to Reinhold et al., 2013)



# **Reference model claystone (Southern Germany)**



- Second model represents Opalinus clay formation in Southern Germany (Mid\_Jurassic\_1)
- Depth of host rock formation: 600-800 m bsl
- Underlying: Jurassic and Keuper
- Overlying: Upper Jurassic, Tertiary
- Karstification of limestone layers
- Model represents geologic conditions of Swabian
  All conductions of Swabian

Alb and comparable regions (Reinhold et al., 2016)



# **Reference model rock salt (stratiform salts)**



- Model focuses on rock salt of the Zechstein (in particular: Straßfurt formation)
- Depth of the host rock: **600-850** m below surface
- Underlying: Zechstein anhydrite and Keuper
- **Overlying**: younger Zechstein succession, Bunter, Cenozioc sedimentary rocks
- Model information are taken from the KOSINA
  project (BGR, 2017)



# **Reference model crystalline rock**



- Crystalline Model in Granite
- Depth of the host rock: < 900 m below surface
- Underlying: -
- **Overlying**: Triassic sediments
- Model represents geology of the mitteldeutsche Kristallinschwelle according to project CHRISTA-II (BGR, 2021)



- Stored as YAML-files, containing most relevant **physical properties** of formations in reference models:
  - Density
  - (Effective) porosity
  - Permeability
  - Heat capacity

- Heat conductivity
- Seismic velocities
- Specific electrical resistivity
- Diffusivity



Synthetic models are based on **Europe-wide studies**:

- **Claystone**: Mont Terri URL (Switzerland), ANDRA URL (France), ANSICHT (Germany)
- **Rock salt**: German salt structures (Gorleben, Asse)
- **Crystalline**: Äspo URL (Sweden), TURVA (Finland)

However, do the synthetic models represent scenarios that are close enough to real geological conditions?

- Detailed research by BGE in two areas (*Gebiete zur Methodenentwicklung*)
- Possibilty to access geological models and adapt for our needs



# **Geophysical modelling – Forward models**

Geophysical forward modelling in

pyGIMLi:

- Performed on geological models (*GemPy-pyGIMLi* link)
- Only **geoelectric** measurements up to this point
- Borehole- or surface-based surveys





Geophysical forward modelling in

pyGIMLi:

- Performed on geological models (*GemPy-pyGIMLi* link)
- Only **geoelectric** measurements up to this point
- Borehole- or surface-based

surveys





# **Geophysical modelling – Forward models**

#### Geophysical forward modelling in

pyGIMLi:

- Performed on geological models (*GemPy-pyGIMLi* link)
- Only **geoelectric** measurements up to this point
- Borehole- or surface-based

surveys





# **Optimal Experimental Design – Theoretical background**



#### "Conventional" data acquisition:

• All electrodes along a survey line are used for measurement (in the case above: 40 electrodes

#### -> 741 data points per time step)

• Includes measurements that contain **no new / relevant information** for measurement



# **Optimal Experimental Design – Theoretical background**

"Compare-R" method:



**RWTHAACHEN** UNIVERSITY

# **Optimal Experimental Design – Theoretical background**

"Compare-R" method (Uhlemann, 2018):

• Uses **resolution matrix** of linearized Gauss-Newton solution for ERT problem; defined as:

 $R = (G^T G + C)^{-1} G^T G$ 

 Iterative optimization starts from a set of base measurements -> calculation of change in resolution matrix for each possible new measurement:

$$\Delta R_b = \frac{z}{1 + (g * z)} (g^T - y^T) \qquad \text{where} \quad z = (G_b^T g_b + C)^{-1} g, \qquad y = (G_b^T G_b) z$$

• All additional measurements are **ranked according to improvement** of resolution matrix:

$$F_{CR} = \frac{1}{m} \sum_{j=1}^{m} \frac{w_{t,j} \,\Delta R_{b,j}}{R_{c,j}}$$

• Depending on chosen step size, **n measurements** with greatest benefit **are added to base set** 



#### "Compare-R" method:

- Provides possibility to **optimize** geoelectrical measurements in **2D and 3D**
- Application to (petrophysical) joint inversions?



#### **Geophysical modelling and OED:**

- Implement CR method and apply to first small-scale experiments
- Implement seismic forward simulations and inversions on reference models
- Work on OED for joint inversion approaches
- Look into other approaches of OED (using Bayesian experimental design)



QIANG, S., SHI, X., KANG, X., & REVIL, A. (2022). Optimized arrays for electrical resistivity tomography survey using Bayesian experimental design. *GEOPHYSICS*, *87*(4), E189–E203. <u>https://doi.org/10.1190/geo2021-0408.1</u>

REINHOLD, K., STARK, L., KÜHLENZ, T., & PTOCK, L. (2016). *Endlagerstandmodell Süd (AnSichT)—Teil 1: Beschreibung des geologischen Endlagerstandmodells* (Ergebnisbericht Nr. 9Y3207000000; F+E Endlagerung, S. 72). Bundesanstalt für Geowissenschaften und Rohstoffe.

UHLEMANN, S., WILKINSON, P. B., MAURER, H., WAGNER, F. M., JOHNSON, T. C., & CHAMBERS, J. E. (2018). Optimized survey design for electrical resistivity tomography: Combined optimization of measurement configuration and electrode placement. *Geophysical Journal International*, *214*(1), 108–121. <u>https://doi.org/10.1093/gji/ggy128</u>

