Improvement of predictive Quality for Final Repository Site Simulations through Optimal Data Acquisition and Smart Monitoring

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

Vertr.-Prof. Florian Wagner

E.ON Energy Research Center

Institute for Applied Geophysics and Geothermal Energy
Faculty of Georesources and Materials Engineering

Maria Fernanda Morales, M.Sc

apl. Prof. Sergey Oladyshkin
Prof. Wolfgang Nowak

University of Stuttgart

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

Qian Chen, M.Sc.

Bachelor:
- Exploration Technology and Engineering (Applied Geophysics) , China University of Petroleum (East China)

Master:
- Applied Geosciences (RWTH Aachen)
- Simulation Sciences (RWTH Aachen)
- Thesis: “Acoustic traveltime tomography of a cryobot’s ambient ice at Langenferner Glacier, Italy ”

Research:
- Autonomous subglacial ice exploration
- Simulation and Modelling for Advanced Robotic Technologies
- Process and impact models

Nino Menzel, M.Sc.

Bachelor:
- Geoscience, Paleontology / Geophysics (University of Cologne)

Master:
- Applied Geoscience (RWTH Aachen)
- Thesis: “Prospection of a small-scal fault system with ERT and SRT surveys”

Research:
- Optimized Experimental Design
- Parameter Estimation (Geophysical Inversion)

Maria Fernanda Morales Oreamuno, M.Sc.

Bachelor:
- Civil Engineering, University of Costa Rica

Master:

- Water Resources Engineering and Management (WAREM), Uni Stuttgart
- Thesis: Bayesian and information theoretic scores for model selection and similarity analysis

Research:
- Bayesian and information theory
- Surrogate model generation
- Optimal deisgn of experiments

Motivation

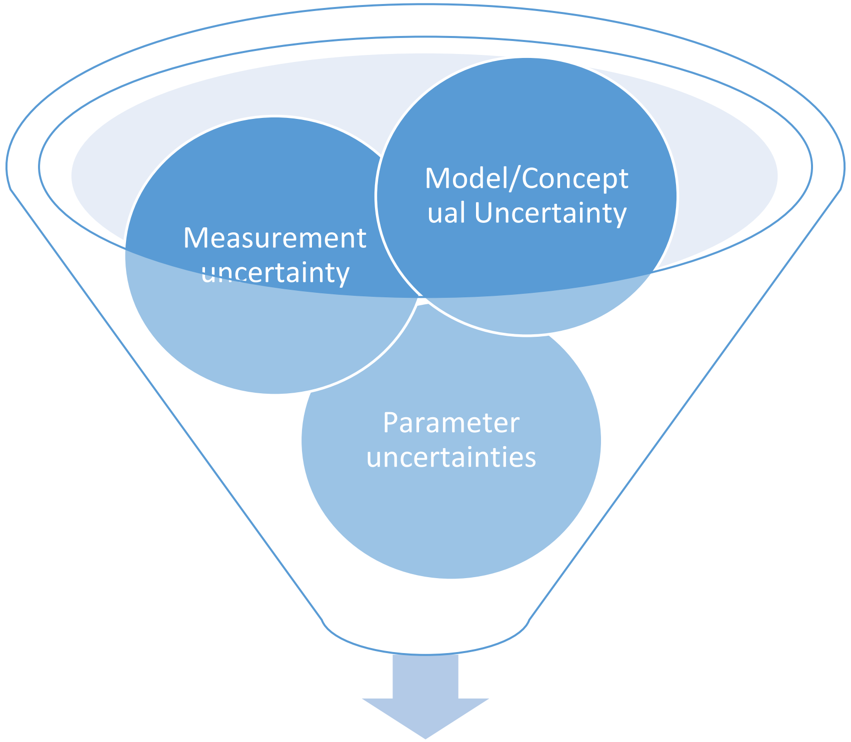
- It is important to **understand the geophysical systems** to be able to use them as a final storage site for radioactive materials

- Build models that can
  - Reproduce current conditions
  - Predict future behaviors under different conditions

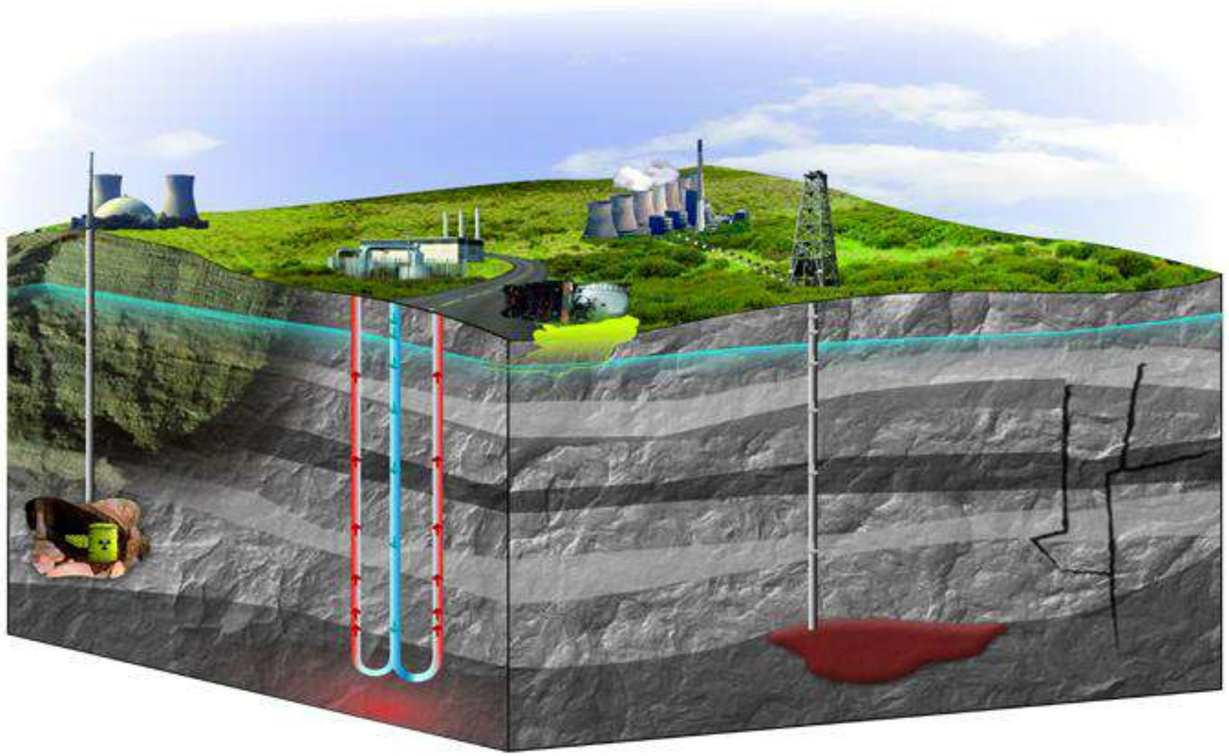
- **Challenge**: Subsurface systems are highly heterogeneous, complex systems and presents non-linear behavior in time and space

Motivation

- **Goal**: Careful and safe operation of nuclear waste disposal sites



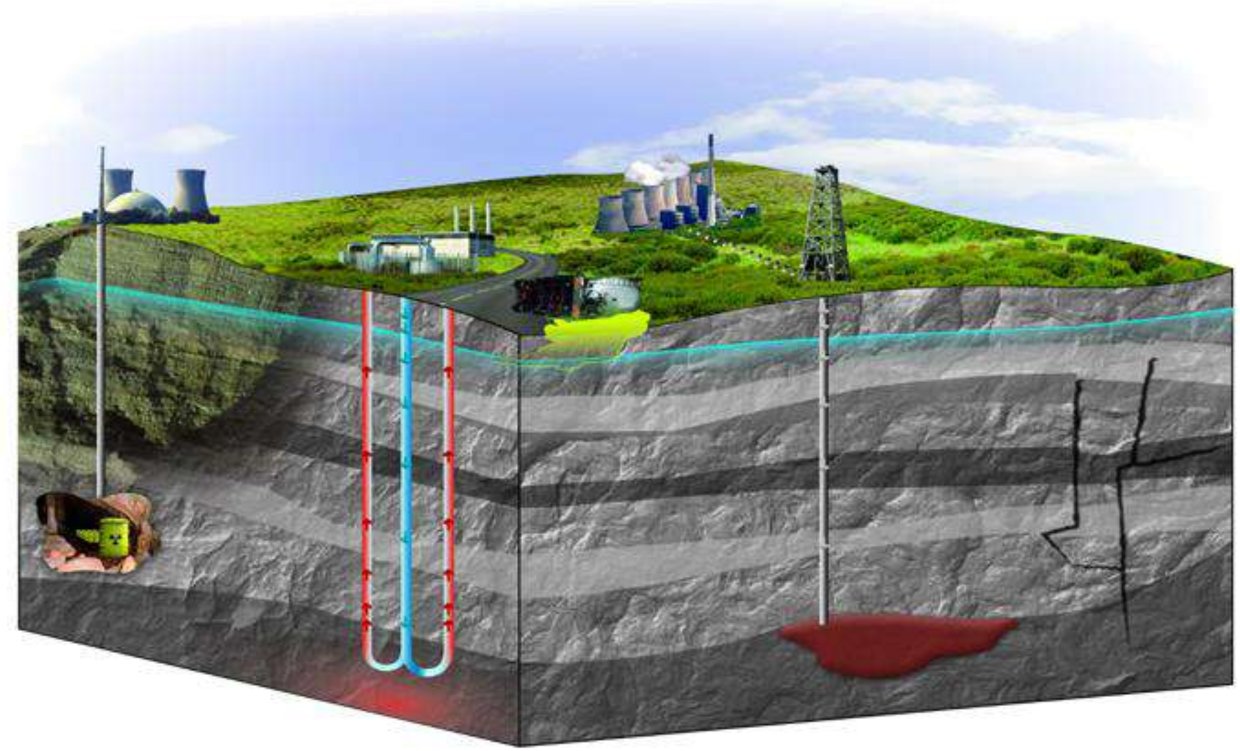
Uncertain predictions



The subsurface is a highly complex geosystem. It is exploited for obtaining natural resources but also storage of anthropogenic waste products like CO2 and radioactive waste.
Source: SimTech@Uni-Stuttgart, 2014

Motivation

- **Measurements** in the study area can help to
  - Improve understanding of the most important processes
  - Determine model/material parameters
  - Reduce model uncertainty
- Measurements of the subsurface are expensive and thus scarce
- Future: plan field measurement campaigns



The subsurface is a highly complex geosystem. It is exploited for obtaining natural resources but also storage of anthropogenic waste products like CO2 and radioactive waste.
Source: SimTech@Uni-Stuttgart, 2014

Which **type** of field measurements provide the greatest information (reduce uncertainty), and **where** and **when** should these measurements be acquired?

Main goals

Implement **methodologies** that allow to determine the most valuable data and monitor a repository .

1. Development and provision of three benchmark scenarios.

2. Improve predictive quality of the models

3. Smart monitoring through process-based optimal design of experiments.

To integrate modern predictive **process and effect modelling**, **Bayesian parameter estimation** and methods of '**Optimal Experimental Design (OED)**' into a modular computer-based workflow.

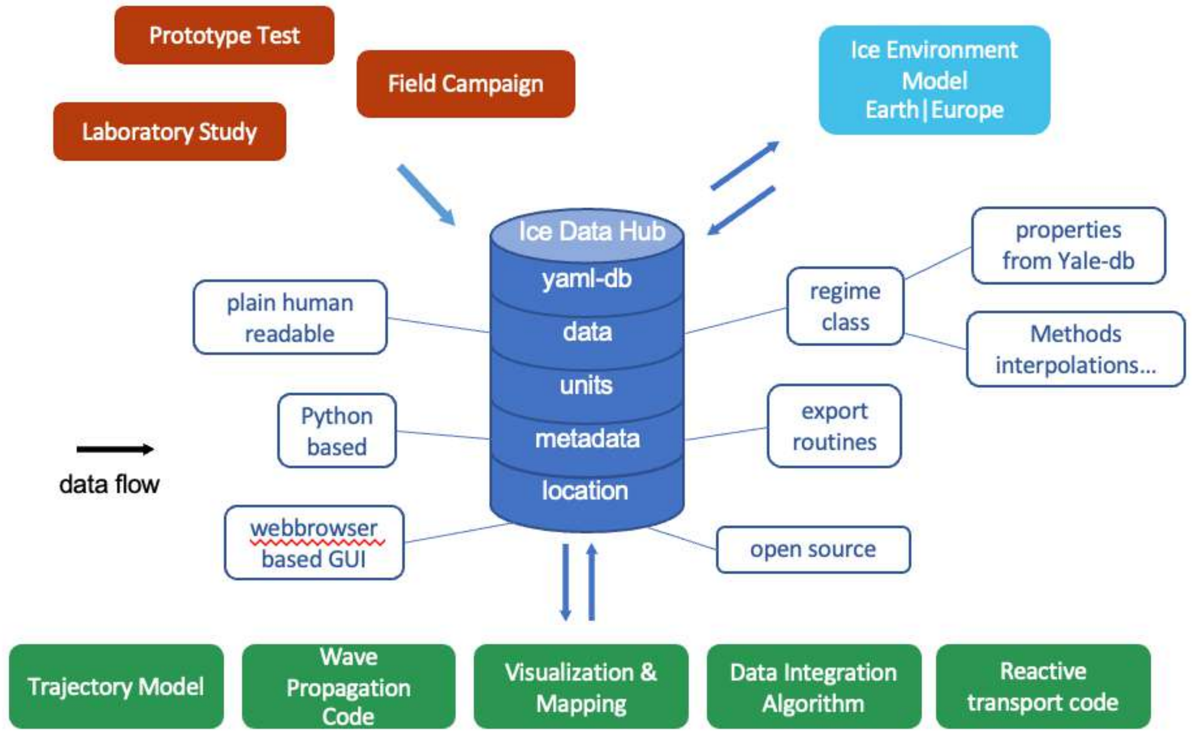
Project workflow

Process model	Impact model	Surrogate model	Geological model	Inverse model
Create reference scenarios, including the geological reference models for each host rocks. Create radionuclide transport model.	The underlying mathematical process model will be extended with regard to selected effect models (the accumulated dose).	Meta-modelling strategy and comparative analysis	Development of a modern and robust parameter estimation and data assimilation based on metamodels and Bayesian active learning	Transferring the developed methods to real geological models

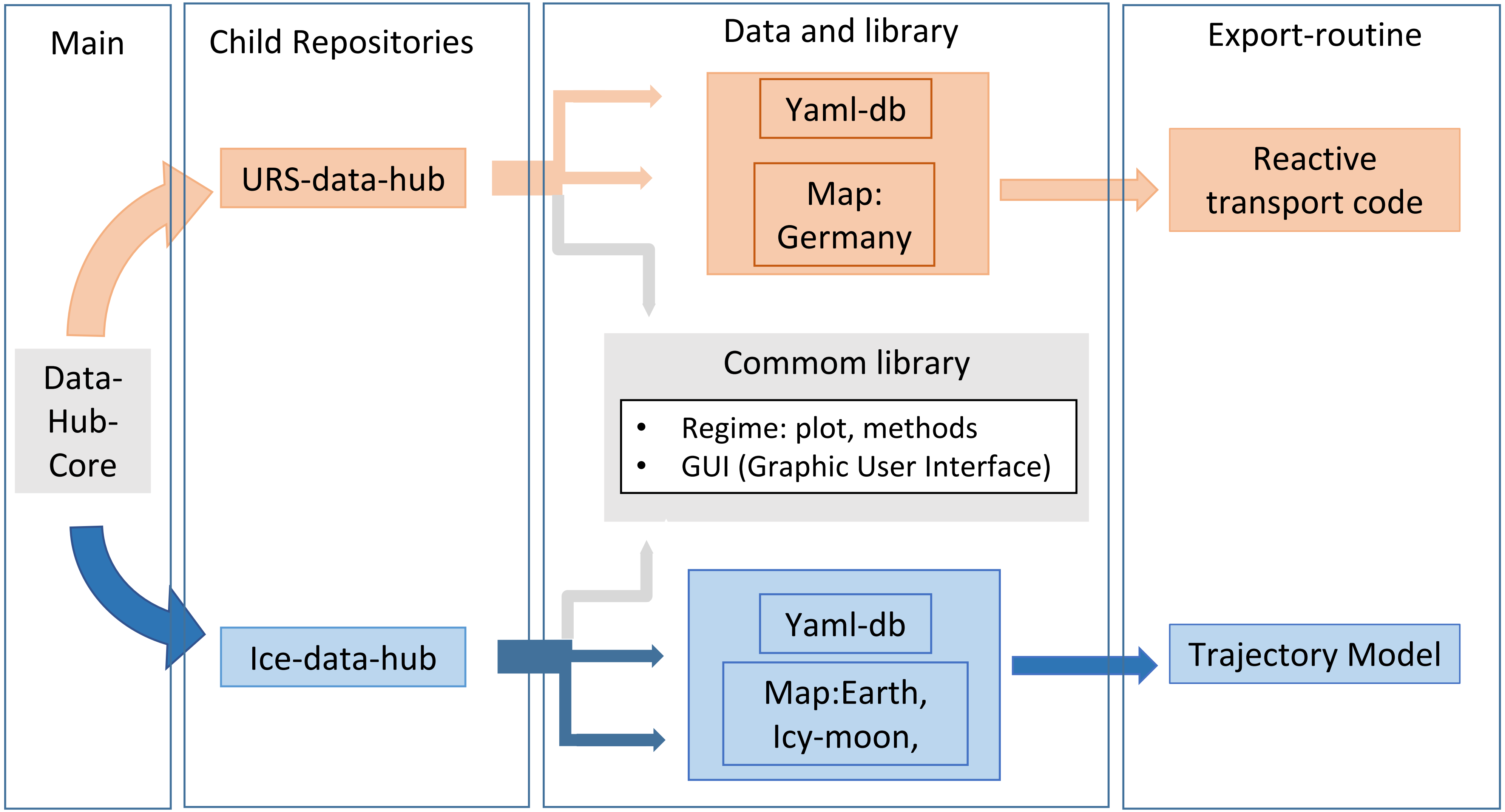
Simulation-ready benchmark scenarios

We create the reference scenarios including the geological reference models for each possible host rocks of a nuclear waste disposal site.

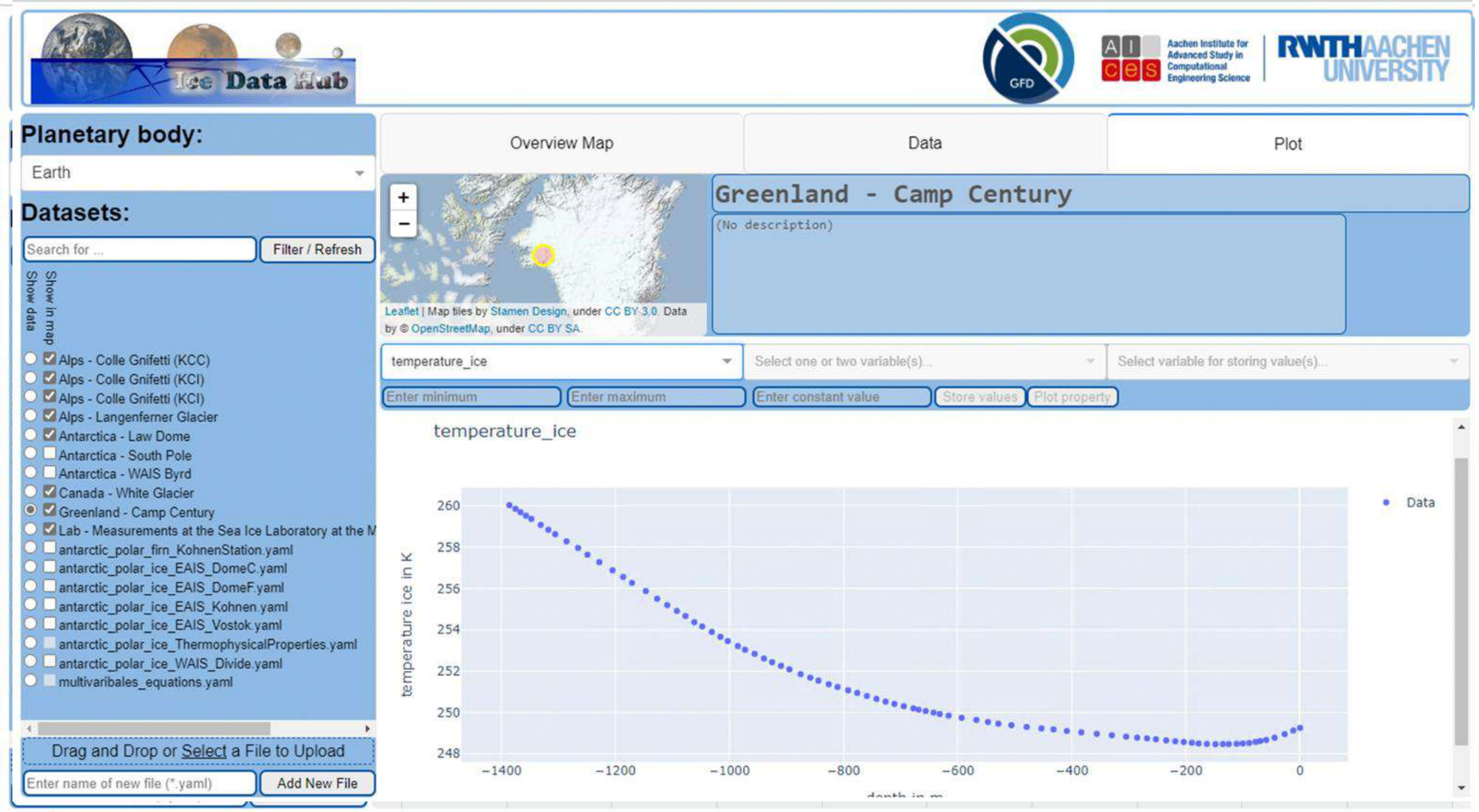
- One geological model will be selected for each reference rock type.
- The material data will be assembled for each benchmark data pool.
- Parametrization of impact scenarios.
- We follow FAIR research data management principles and realize open access.



Structure of Data-Hub-Core



GUI


Ice Data Hub
GFD
AICES Aachen Institute for Advanced Study in Computational Engineering Science
RWTH AACHEN UNIVERSITY
Planetary body:
Earth
Datasets:
Search for ...
Filter / Refresh
Show data
Show in map
Alps - Colle Gnifetti (KCC)
Alps - Colle Gnifetti (KCI)
Alps - Colle Gnifetti (KCI)
Alps - Langenferner Glacier
Antarctica - Law Dome
Antarctica - South Pole
Antarctica - WAIS Byrd
Canada - White Glacier
Greenland - Camp Century
Lab - Measurements at the Sea Ice Laboratory at the M
antarctic_polar_firn_KohnenStation.yaml
antarctic_polar_ice_EAIS_DomeC.yaml
antarctic_polar_ice_EAIS_DomeF.yaml
antarctic_polar_ice_EAIS_Kohnen.yaml
antarctic_polar_ice_EAIS_Vostok.yaml
antarctic_polar_ice_ThermophysicalProperties.yaml
antarctic_polar_ice_WAIS_Divide.yaml
multivaribales_equations.yaml
Drag and Drop or Select a File to Upload
Enter name of new file (*.yaml)
Add New File
Overview Map
Data
Plot
Leaflet | Map tiles by Stamen Design, under CC BY 3.0. Data by © OpenStreetMap, under CC BY SA.
Greenland - Camp Century
(No description)
temperature_ice
Select one or two variable(s)...
Select variable for storing value(s)...
Enter minimum
Enter maximum
Enter constant value
Store values
Plot property
temperature_ice
temperature ice in K
Data
260
258
256
254
252
250
248
−1400
−1200
−1000
−800
−600
−400
−200
0

GUI

Rock type:

Crystalline

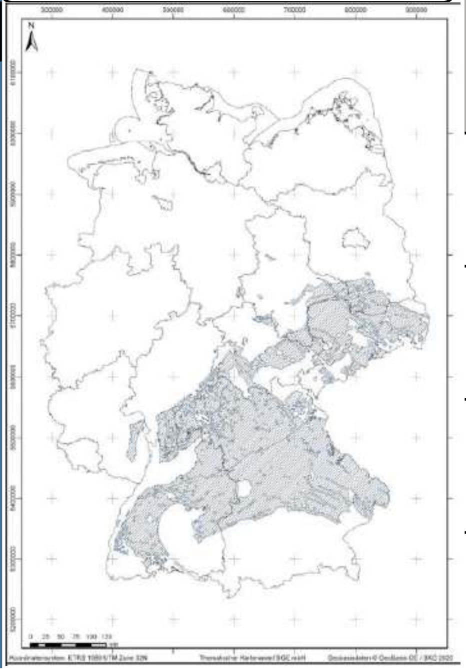
Datasets:

- ❑ Transport parameters
- ❑ Geological model
- ❑ …

.
.
.

Add New File .yaml

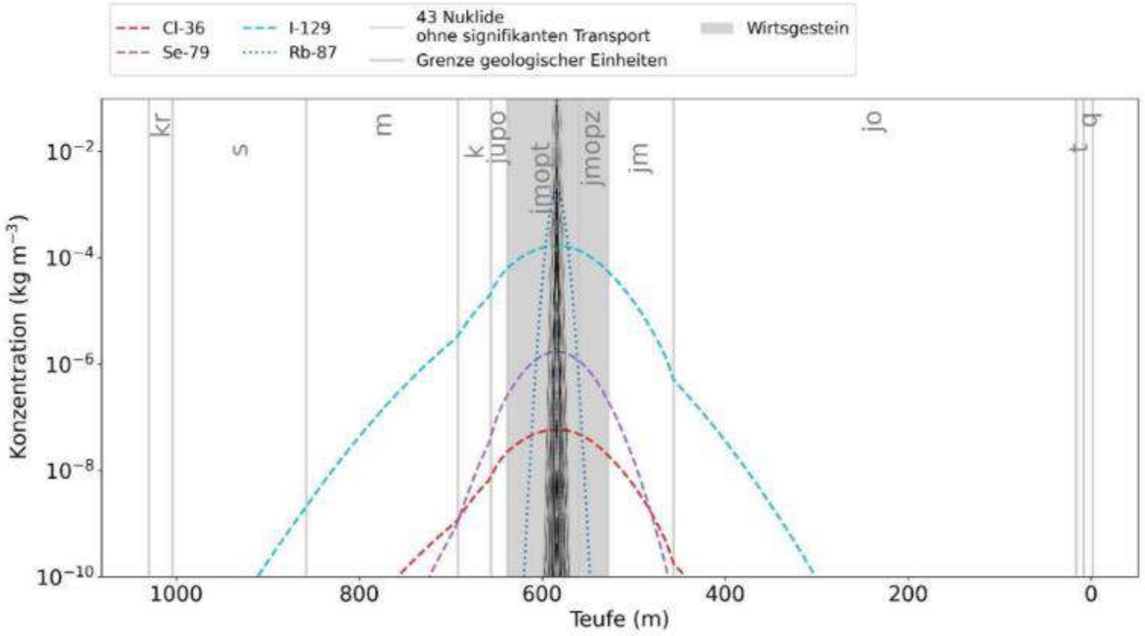
Overview Map



Data | export

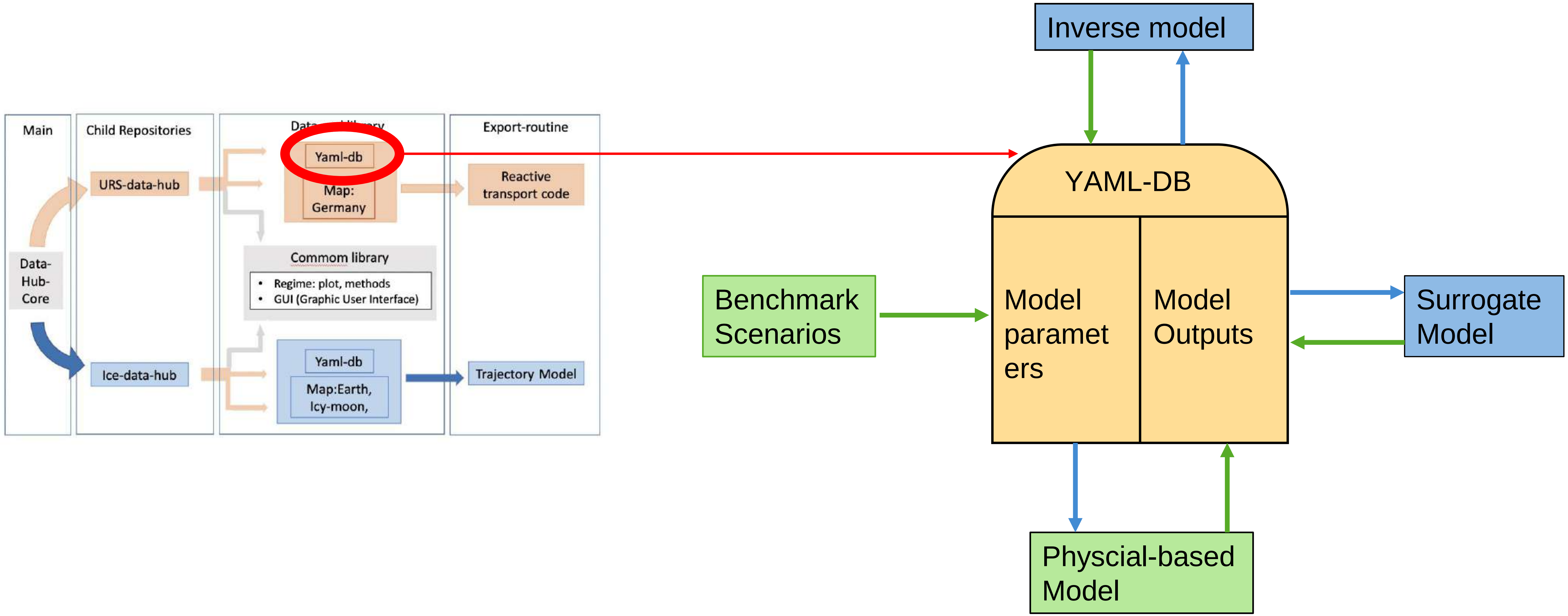
Property	…
permeability	
porosity	
tortuosity	
…	

Plot



(Sub-areas Interim Report, 2020, BGE)
(SG02303/97-2/2-2022#10 – Objekt-ID: 919256 – Revision: 00)

Data exchange interface



Hydrothermal process and impact models

Process model

Reactive transport code:

+ Groundwater Flow
+ Diffusion
+ Reaction

Impact model

accumulated radiation dose

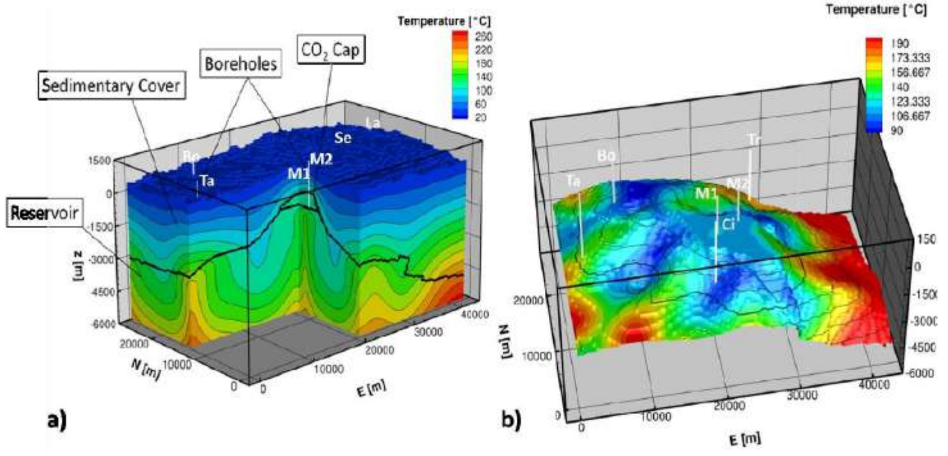
Numerical solver:

- SHEMAT-Suite

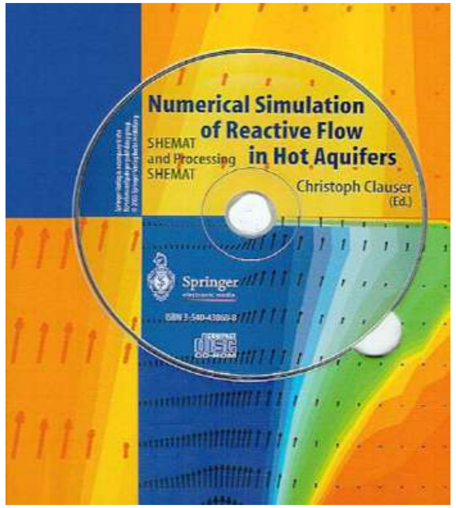
or

- OpenGeoSys

OpenGeoSys
OPEN-SOURCE MULTI-PHYSICS

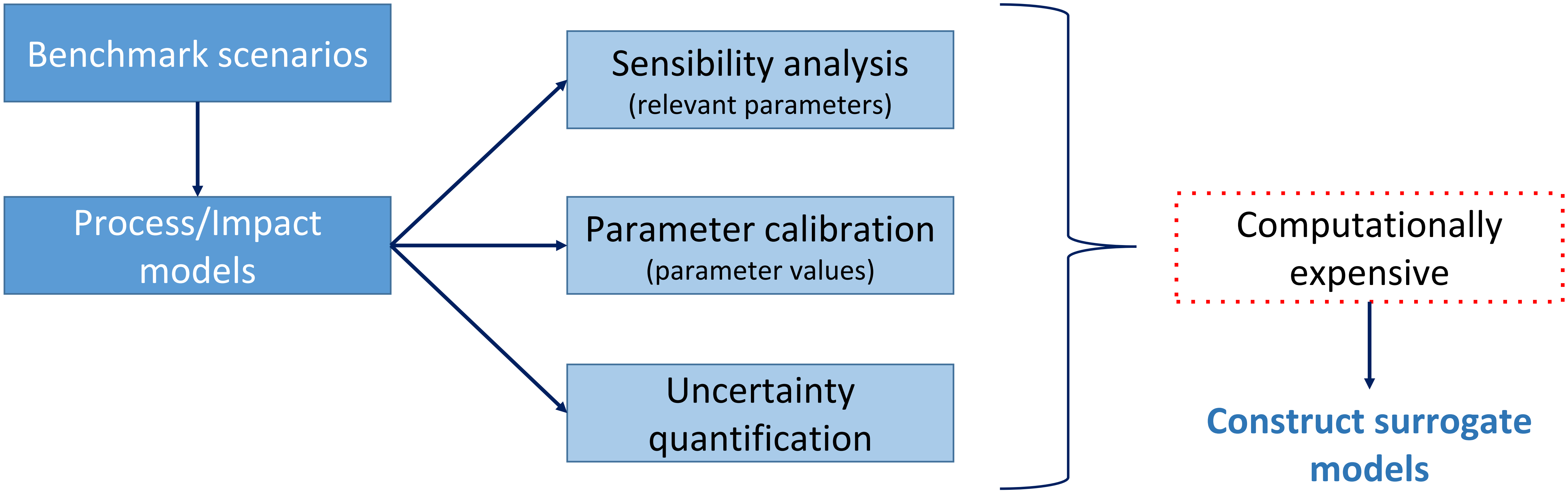


(2022 Standorttage)



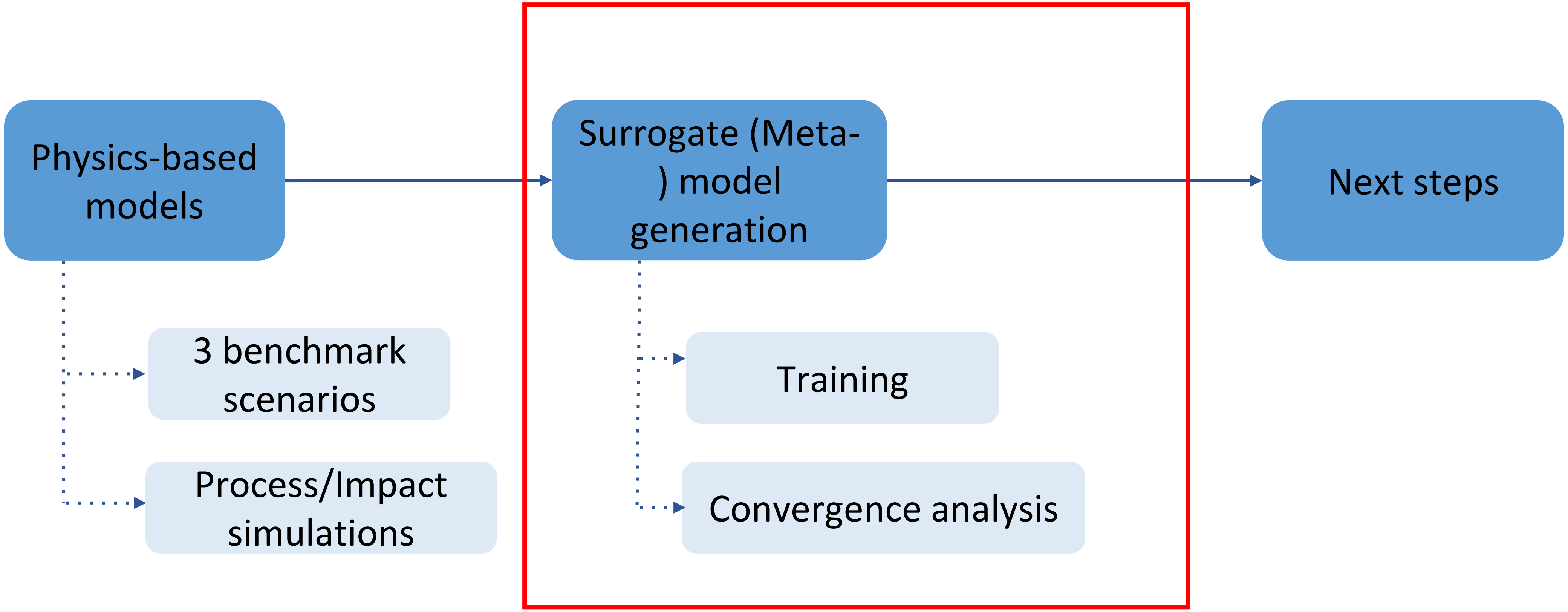
(Clauser 2003)

Surrogate modelling

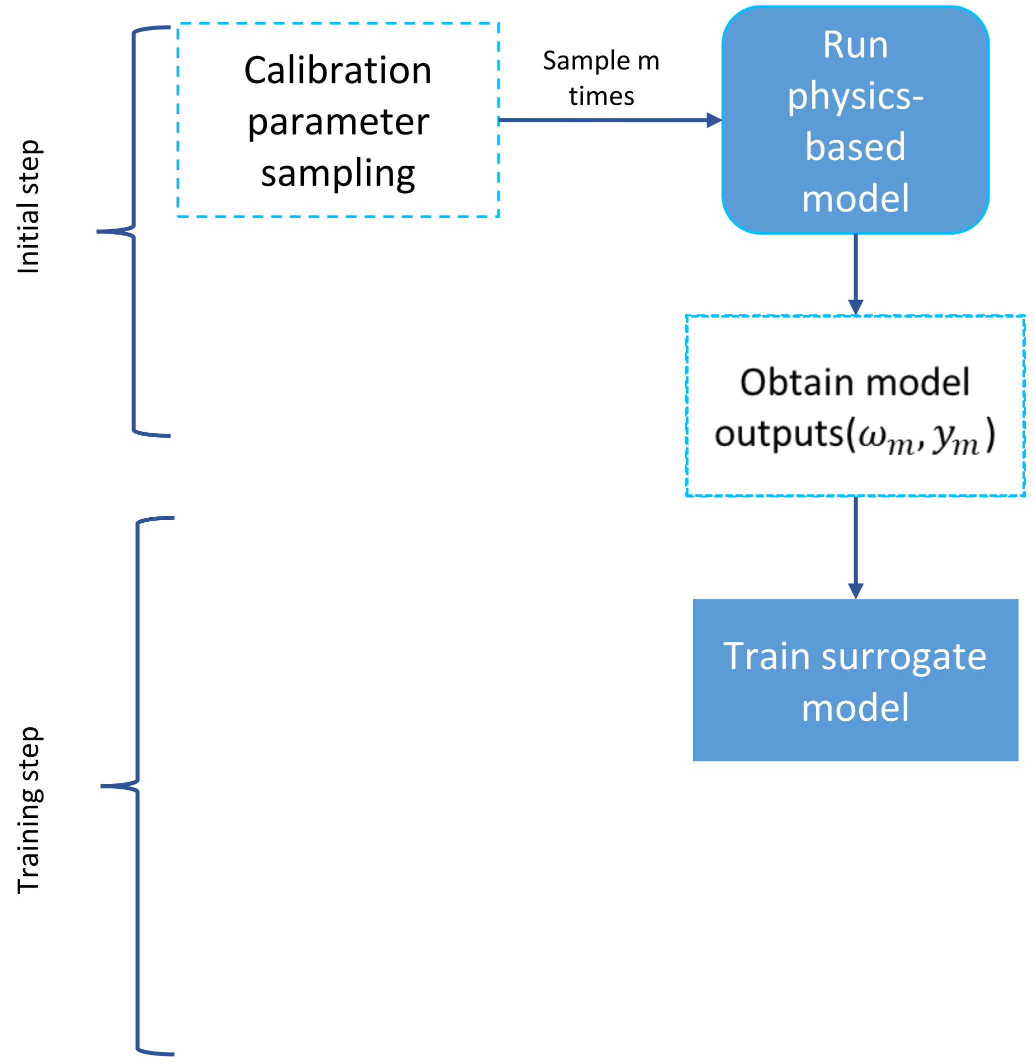


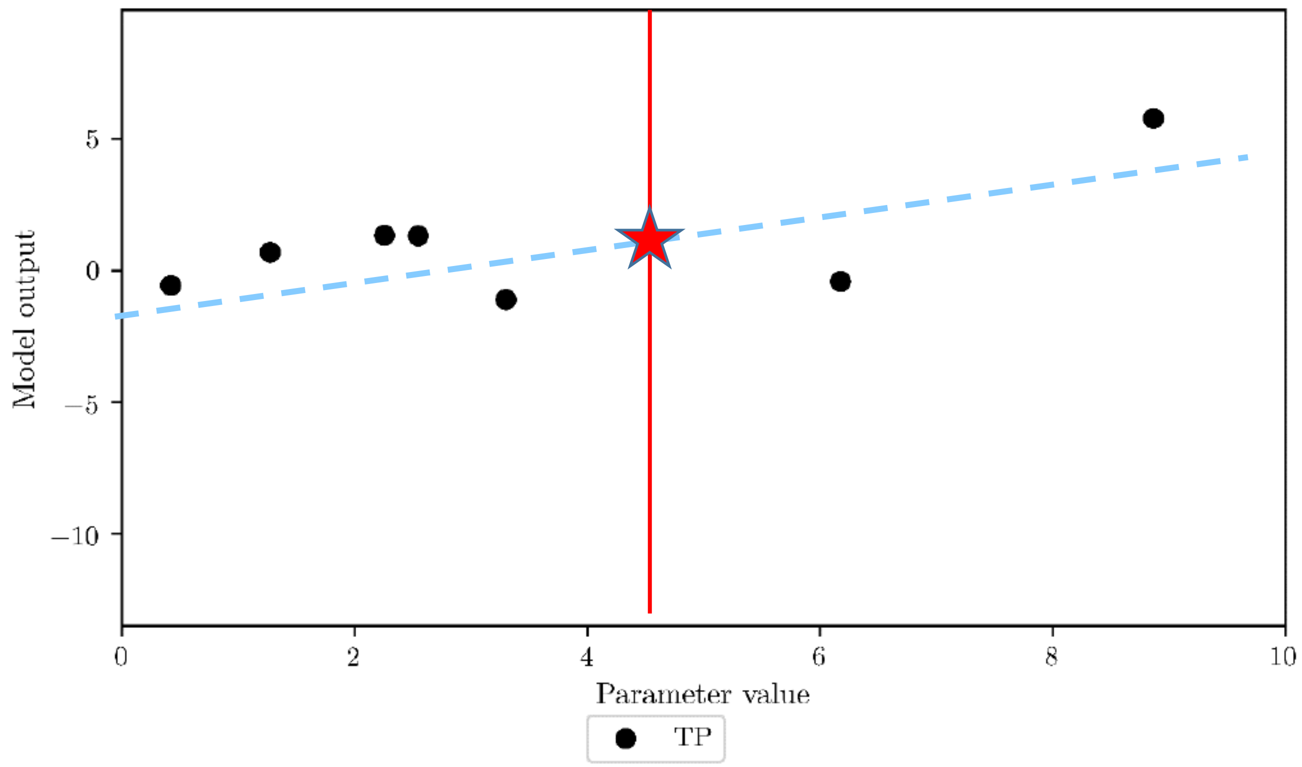
Surrogate modelling

- Statistical approximation of a full-complexity (physics-based) numerical model
  - Trained using the full-complexity model to reproduce its outputs
  - Runs in a fraction of the time



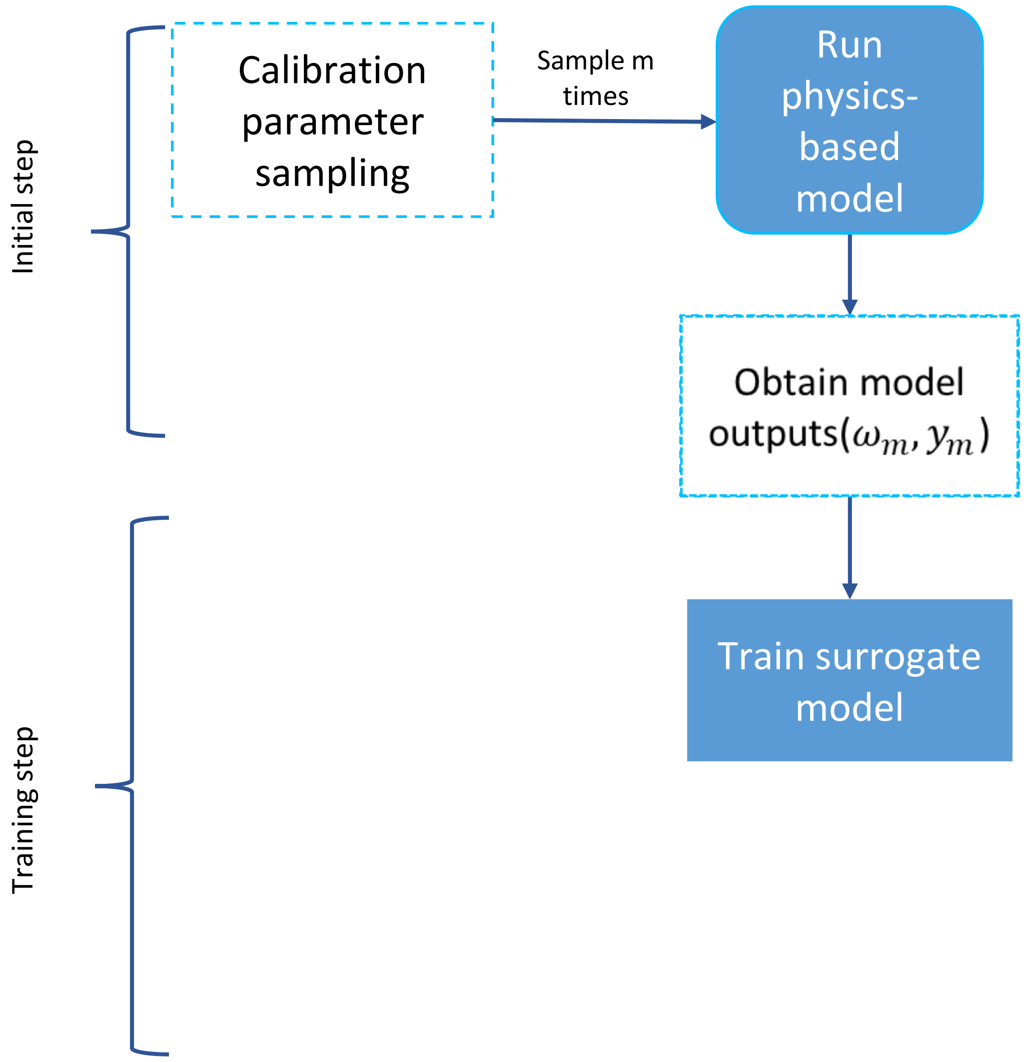
Surrogate Modelling

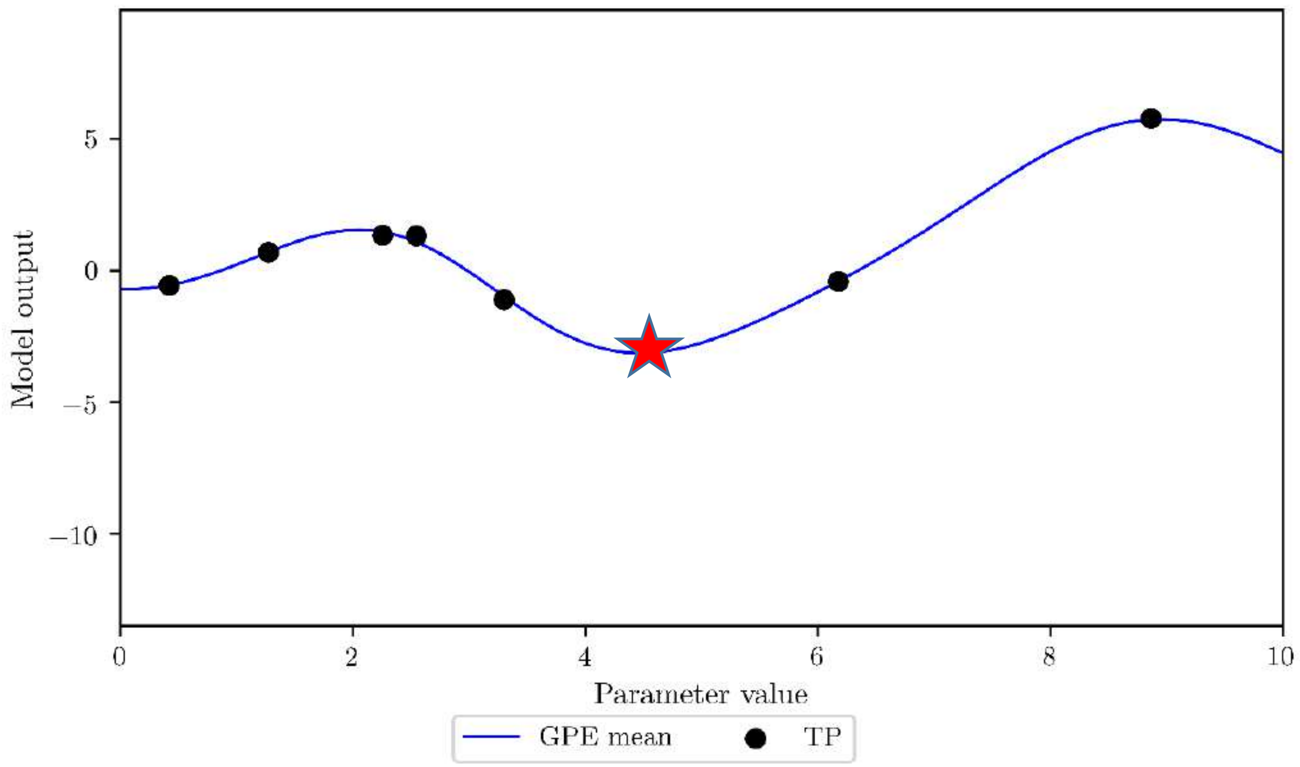




Training point generation for a 1D input – 1D output scenario

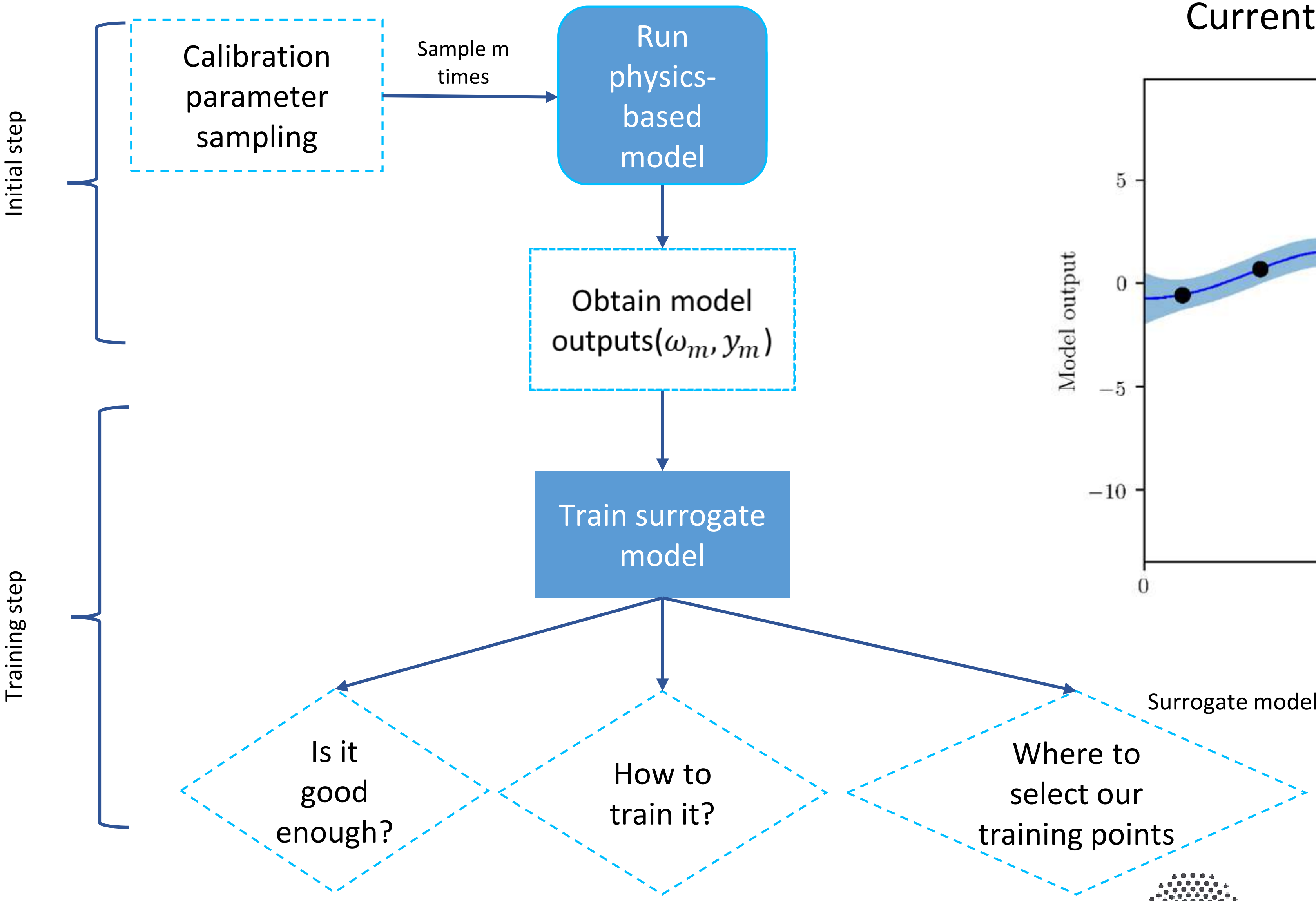
Surrogate Modelling



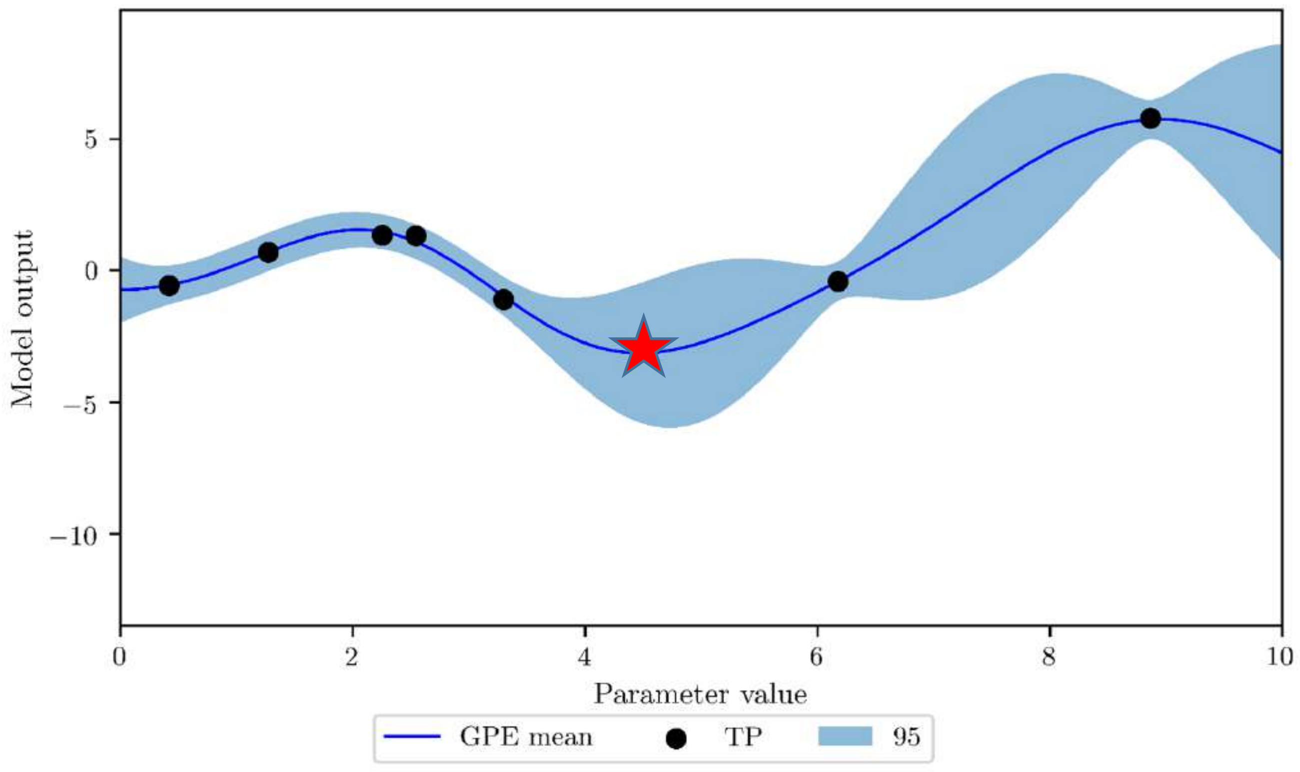


Surrogate model generation based on training points using a Gaussian process regression approach

Surrogate Modelling

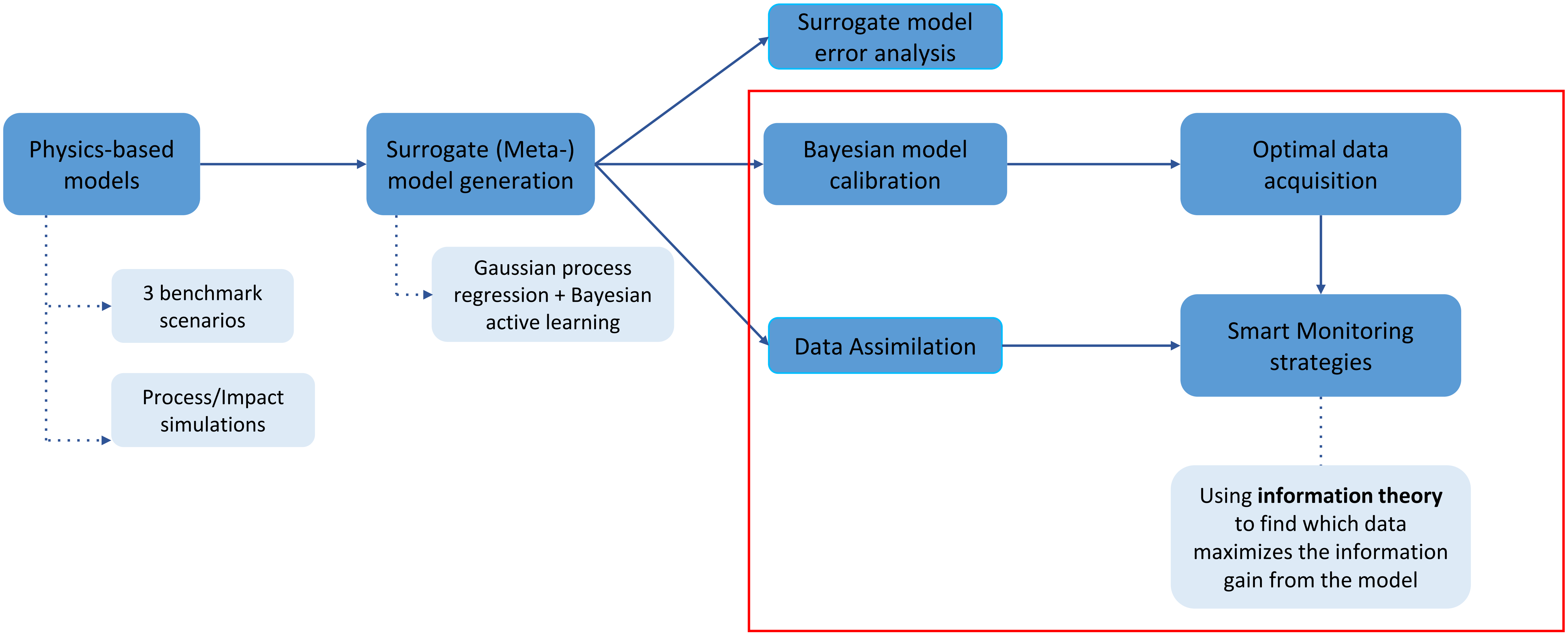


Current approach: Gaussian process regression

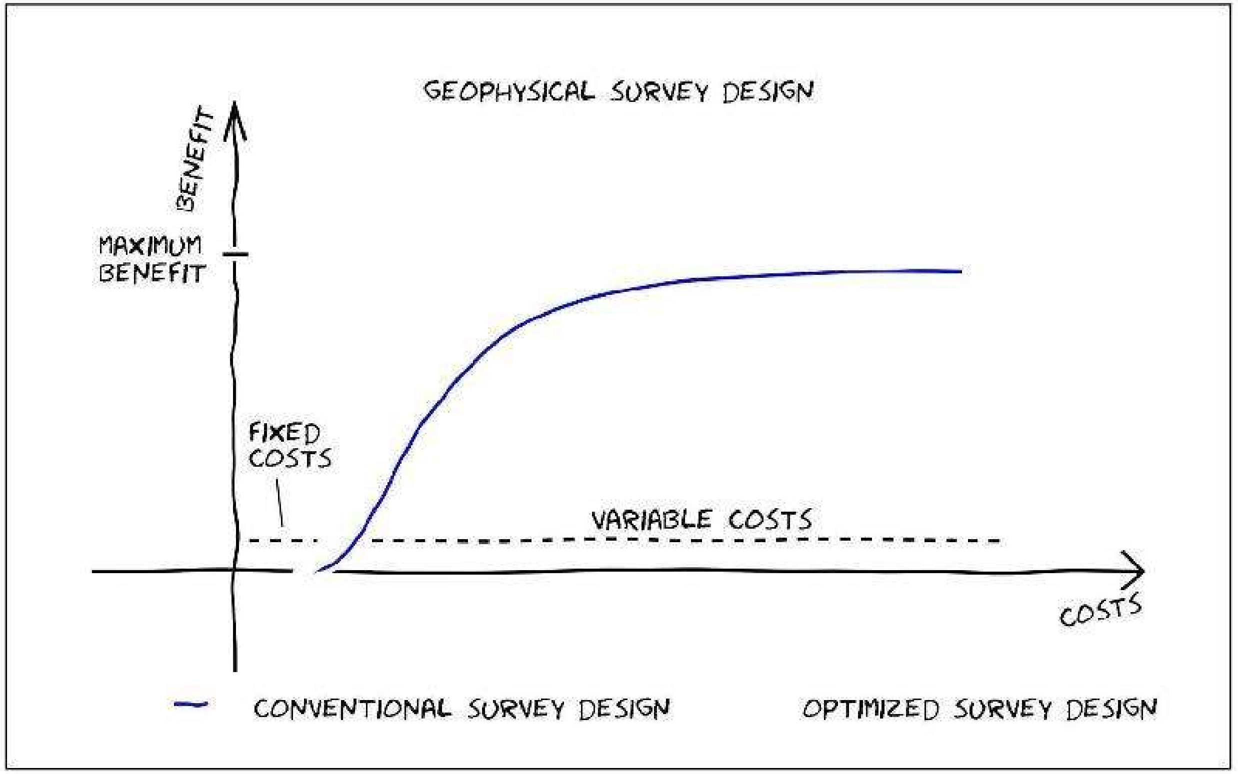


Surrogate model generation with confidence intervals based on training points using a Gaussian process regression approach

Surrogate modelling: next steps



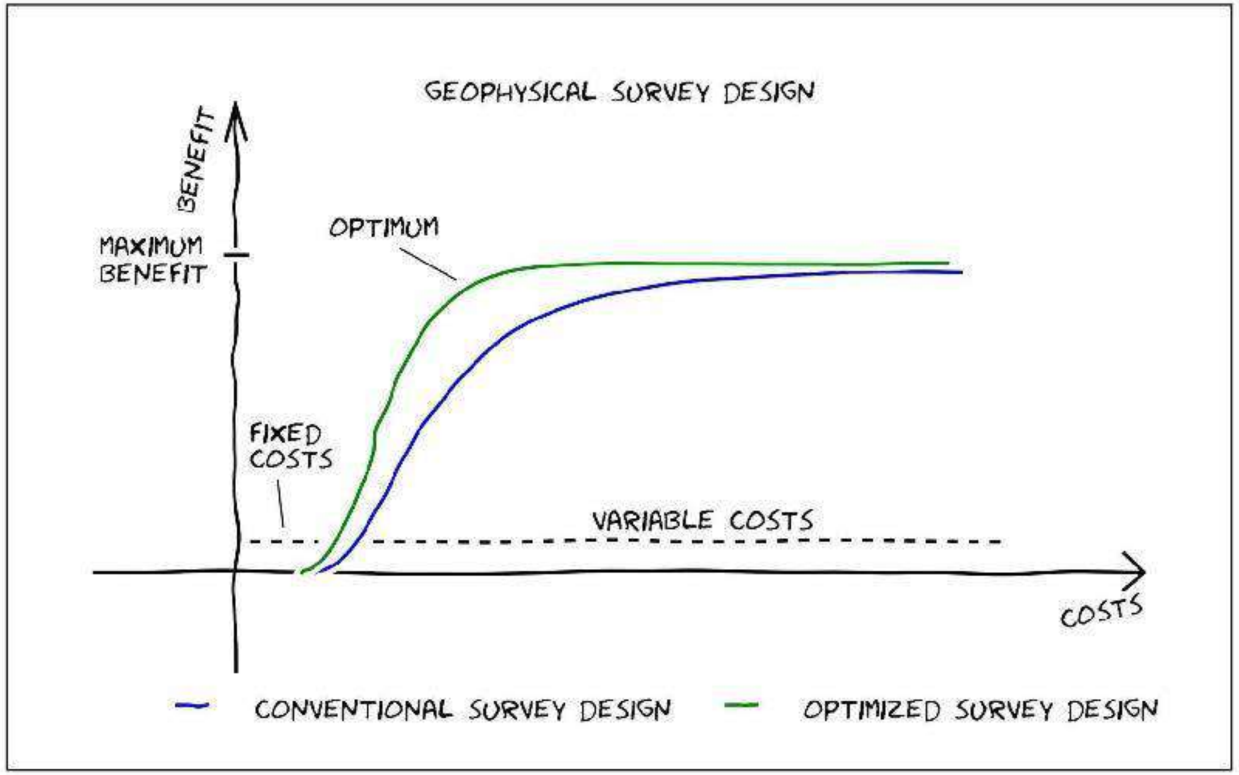
Geophysical inversion – Optimal survey design



Following Maurer, 2010

- **Optimal survey design**
  - Data processing can compensate for missing or inadequate data only to a certain extent
  - Survey optimization aims at **optimizing the information content** of (geo)physical data sets
  - **Limit amount of data** without (drastically) reducing their information content

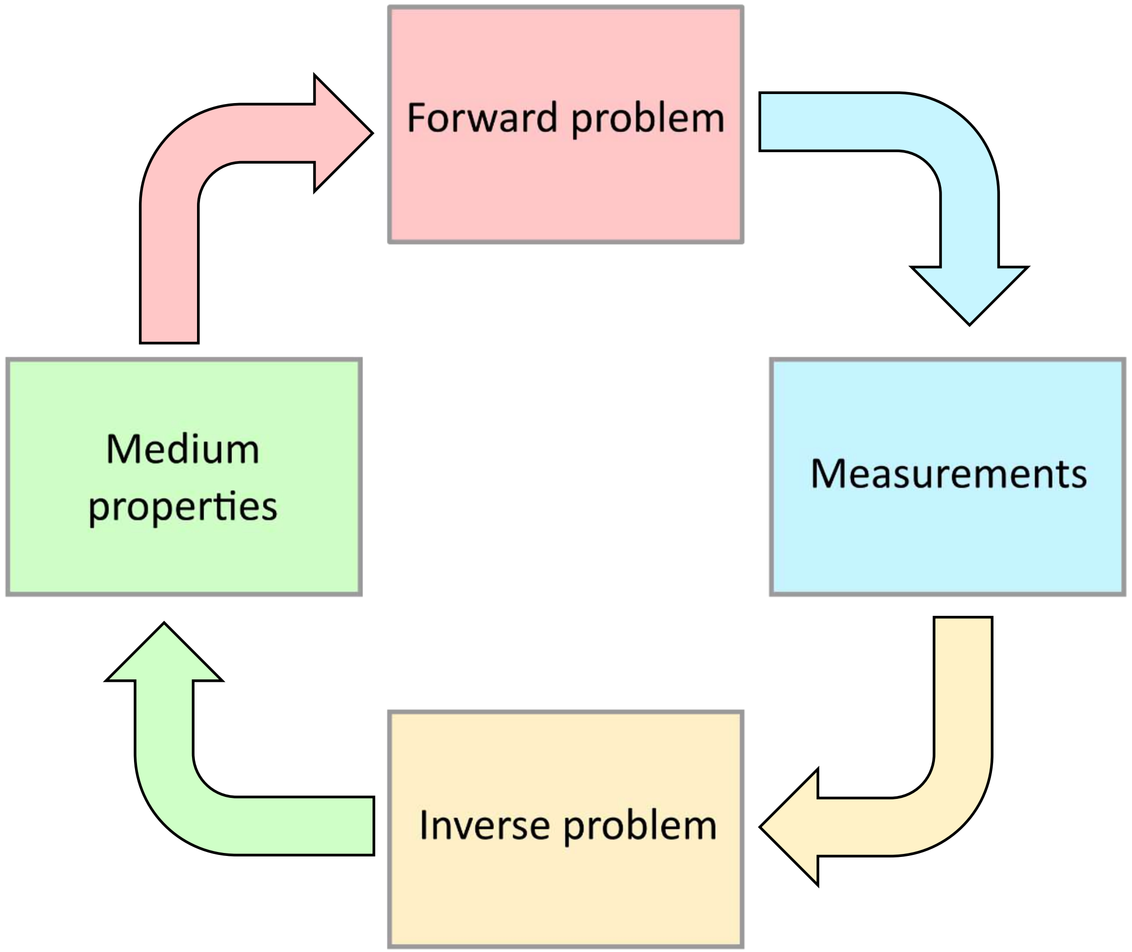
Geophysical inversion – Optimal survey design



Following Maurer, 2010

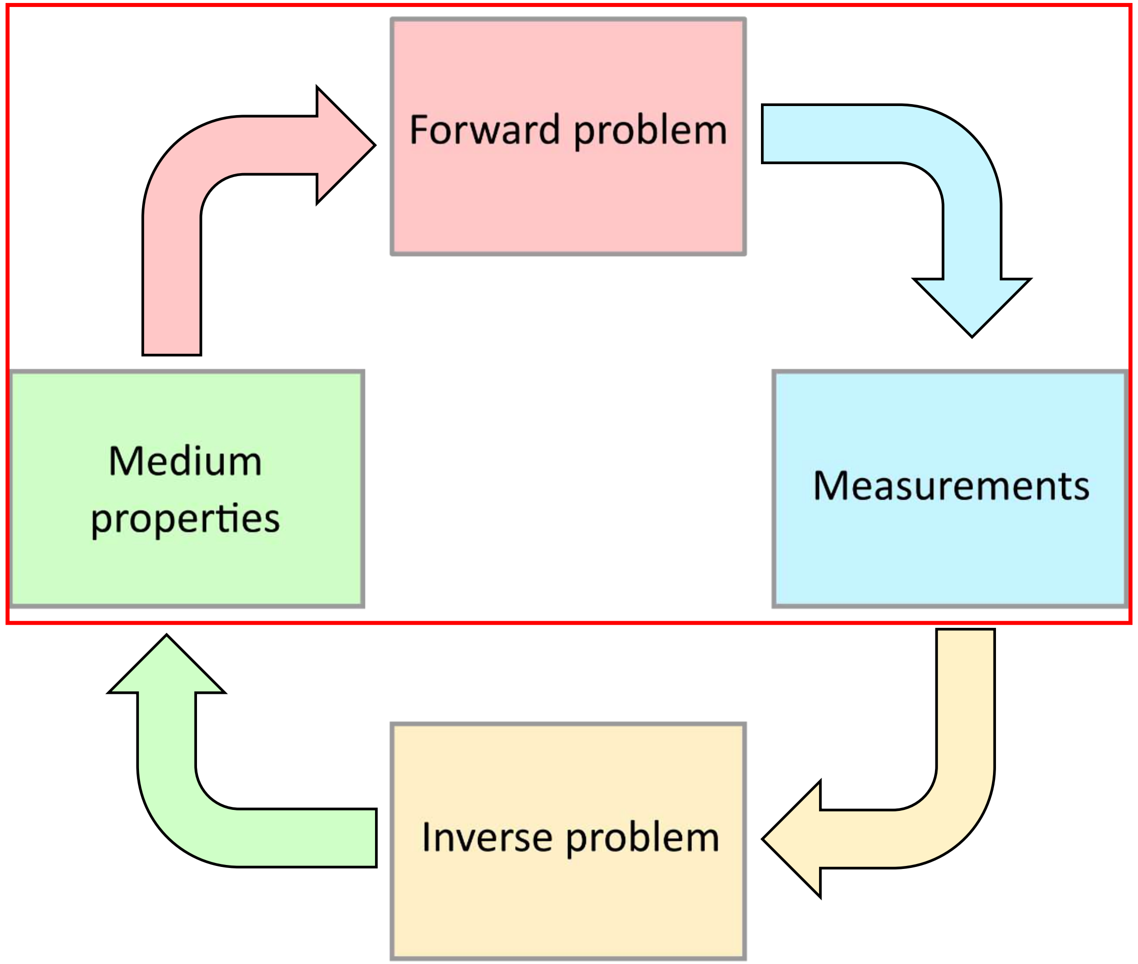
- **Optimal survey design**
  - Data processing can compensate for missing or inadequate data only to a certain extent
  - Survey optimization aims at **optimizing the information content** of (geo)physical data sets
  - **Limit amount of data** without (drastically) reducing their information content

Geophysical inversion - Forward vs. inverse problem



$$d = f(m) + \varepsilon$$

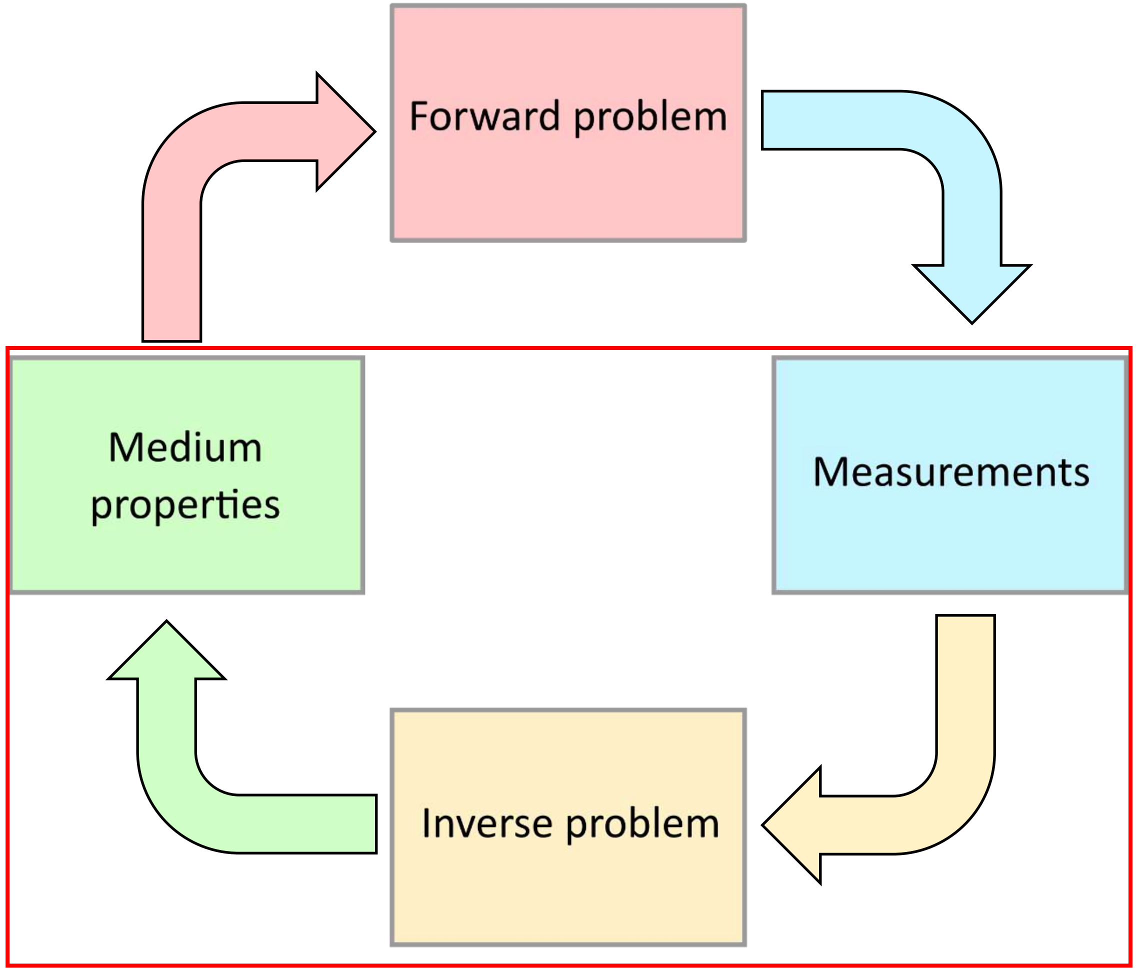
Geophysical inversion - Forward vs. inverse problem



$$d = f(m) + \varepsilon$$

- **Forward modelling:**
  Prediction of observations/data **d** with given model parameters **m**.

Geophysical inversion - Forward vs. inverse problem



$$d = f(m) + \varepsilon$$

- **Forward modelling:**
  Prediction of observations/data **d** with given model parameters **m**.

- **Inverse modelling:**
  Estimation of model parameters **m** with given observations/data **d**.

Geophysical inversion – Common problems

- **Existence of a solution** *(Does any model fit the data?)*

  The observed dataset d cannot be reproduced due to incomplete / wrong model or missing observation errors ε.

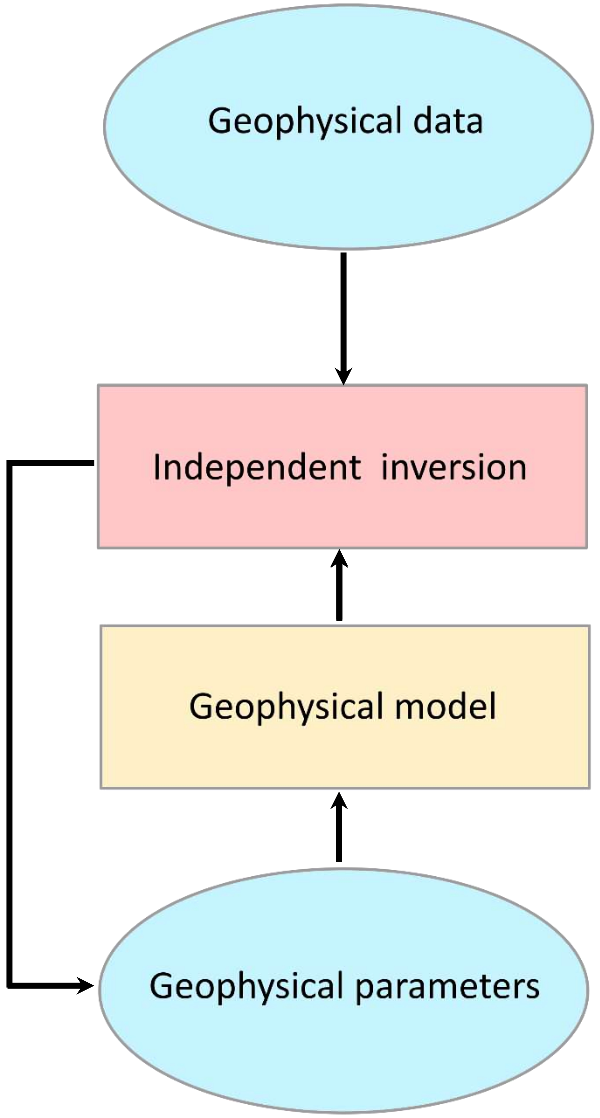
- **Uniqueness of a solution** *(Is there a unique model that describes the data?)*

  In many cases, an infinite number of solutions for m lead to the same observations d.

- **Instabilities of the model** *(Can small changes in d influence the model in a drastic way?)*

  Small observation errors may lead to large changes in the estimated model parameters m.

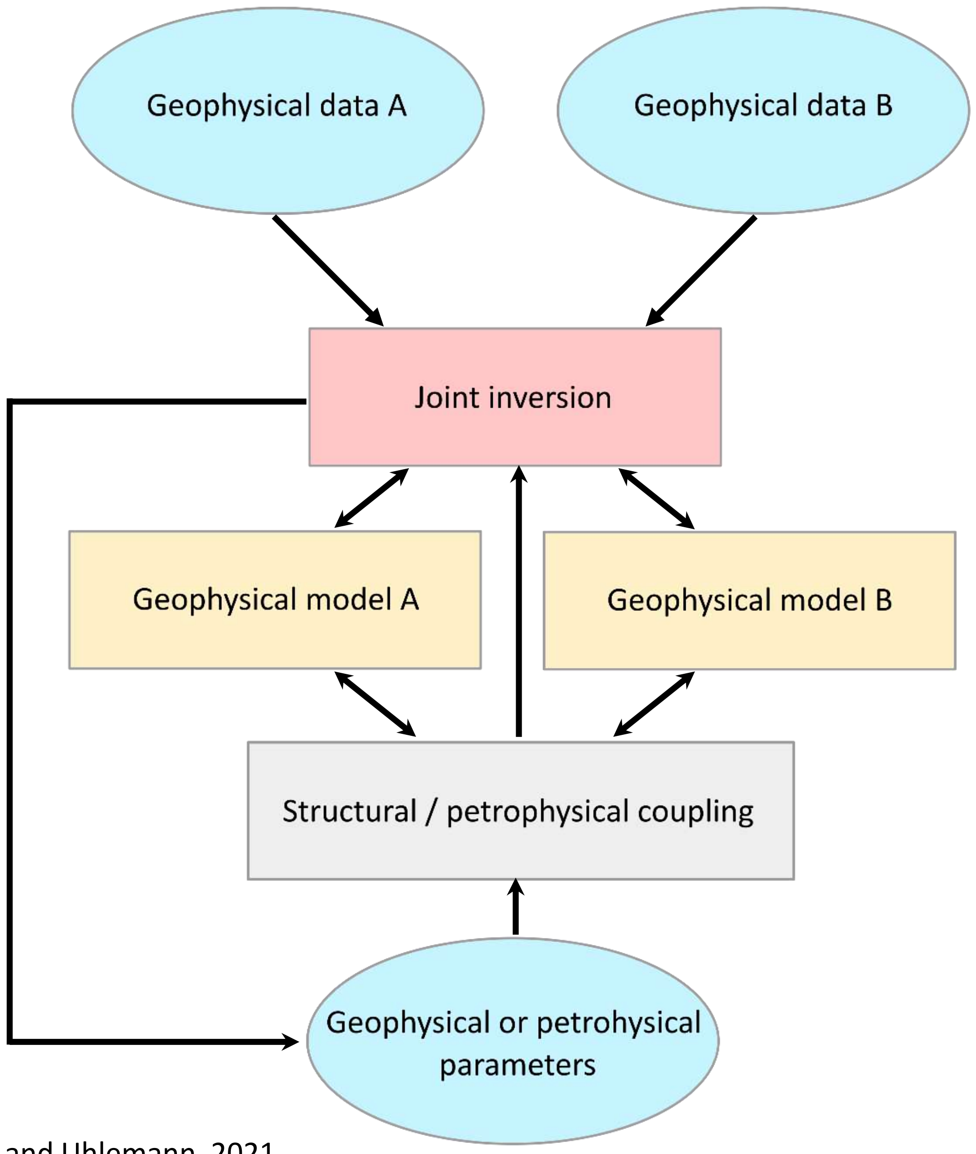
Geophysical inversion – Different approaches



- **Independent inversion:**
  - Geophysical data of one geophysical method
  - Result of inversion is single set of geophysical parameters
  - Inversion independent of other geophysical methods
  - Geophysical forward model needed for link between model parameters and response

Wagner and Uhlemann, 2021

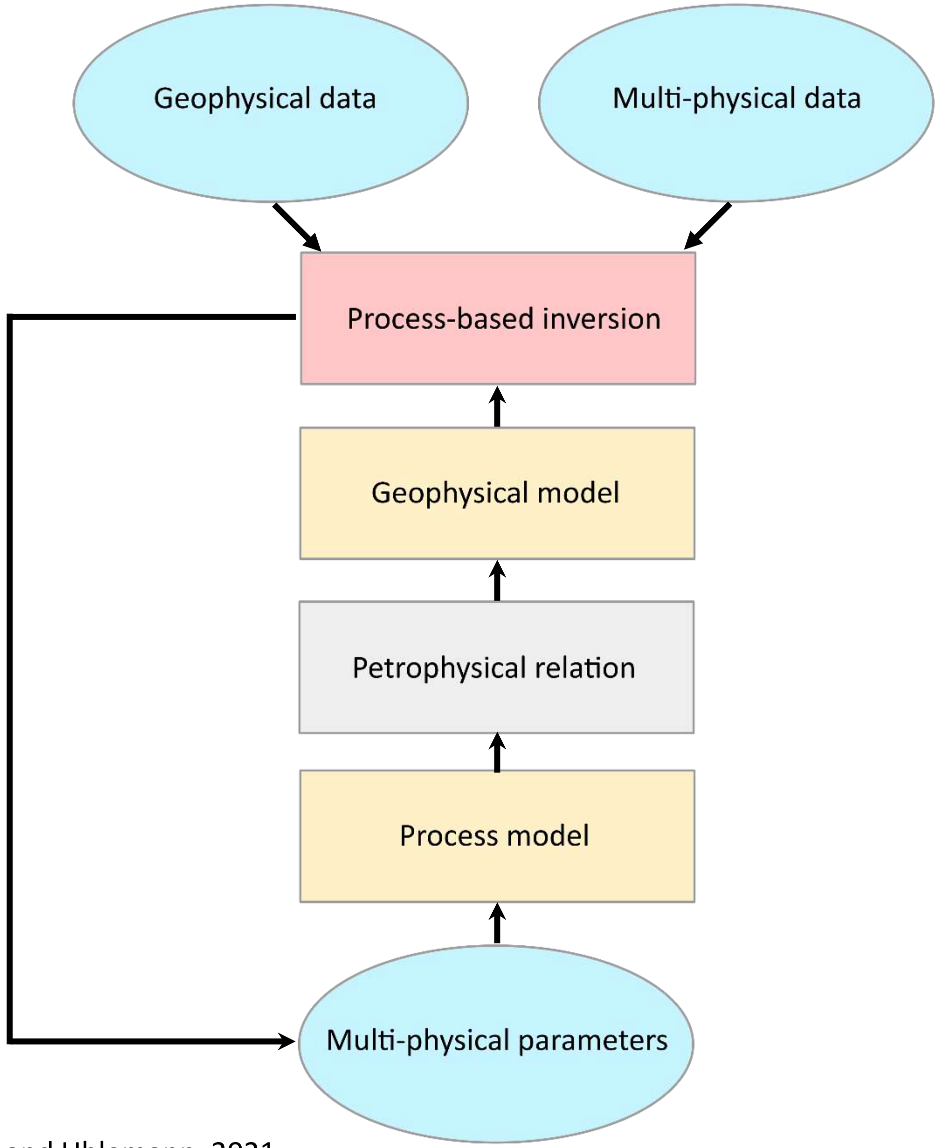
Geophysical inversion – Different approaches



Wagner and Uhlemann, 2021

- **Joint inversion:**
  - Combines multiple geophysical methods in one single parameter estimation
  - **Assumption**: multiple geophysical methods exhibit spatial changes at similar locations in the subsurface
  - *single-property* and *multi-property* joint inversion

Geophysical inversion – Different approaches



Wagner and Uhlemann, 2021

- **Process-based inversion:**
  - Not only based on geophysical parameter estimations
  - allows combination of both geophysical and non-geophysical observations
  - takes dynamic physical process into account
  - success strongly depends on petrophysical relation used

Geophysical inversion - Summary

- Which (geo)physical parameters are most important and how can we optimize the surveys (maximize information content of measurements)?
  - Which measurements are most useful for which host rock?

- “Test” geophysical inversion methods on surrogate models
  - Allows computationally efficient optimization of inversion to improve model quality

End goal

- Measurement introduced in different sub-tasks to improve model prediction

- Implement the workflow and Bayesian inversion methodologies to plan future field campaigns:
  - What type of measurements
  - When and where to locate them

  }
  - Save and optimize resources
  - Reduce modelling uncertainty

- A strategy of monitoring: Maximize storage of radionuclides in the repository.

Thank you for your attention!

Qian Chen, M.Sc.

chen@mbd.rwth-aachen.de

Nino Menzel, M.Sc.

Nino.Menzel@rwth-aachen.de

Maria Fernanda Morales Oreamuno, M.Sc.

maria.morales@iws.uni-stuttgart.de