Verbesserung der prädiktiven Güte endlagerrelevanter Simulationen durch optimale Datenakquise und Smart-Monitoring

Prof. Julia Kowalski

Prof. Florian Wagner

apl. Prof. Sergey Oladyshkin

Dr. Marc S. Boxberg

Prof. Wolfgang Nowak

Qian Chen, M.Sc

Nino Menzel, M.Sc

Maria Fernanda Morales, M.Sc

MBD | RWTH AACHEN UNIVERSITY

Chair of Methods for Model-based Development in Computational Engineering
Faculty of Mechanical Engineering

GIM | RWTH AACHEN UNIVERSITY

Geophysical Imaging and Monitoring Teaching and Research Unit, Faculty of Georesources and Materials Engineering

University of Stuttgart | LS³

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

Table of Contents

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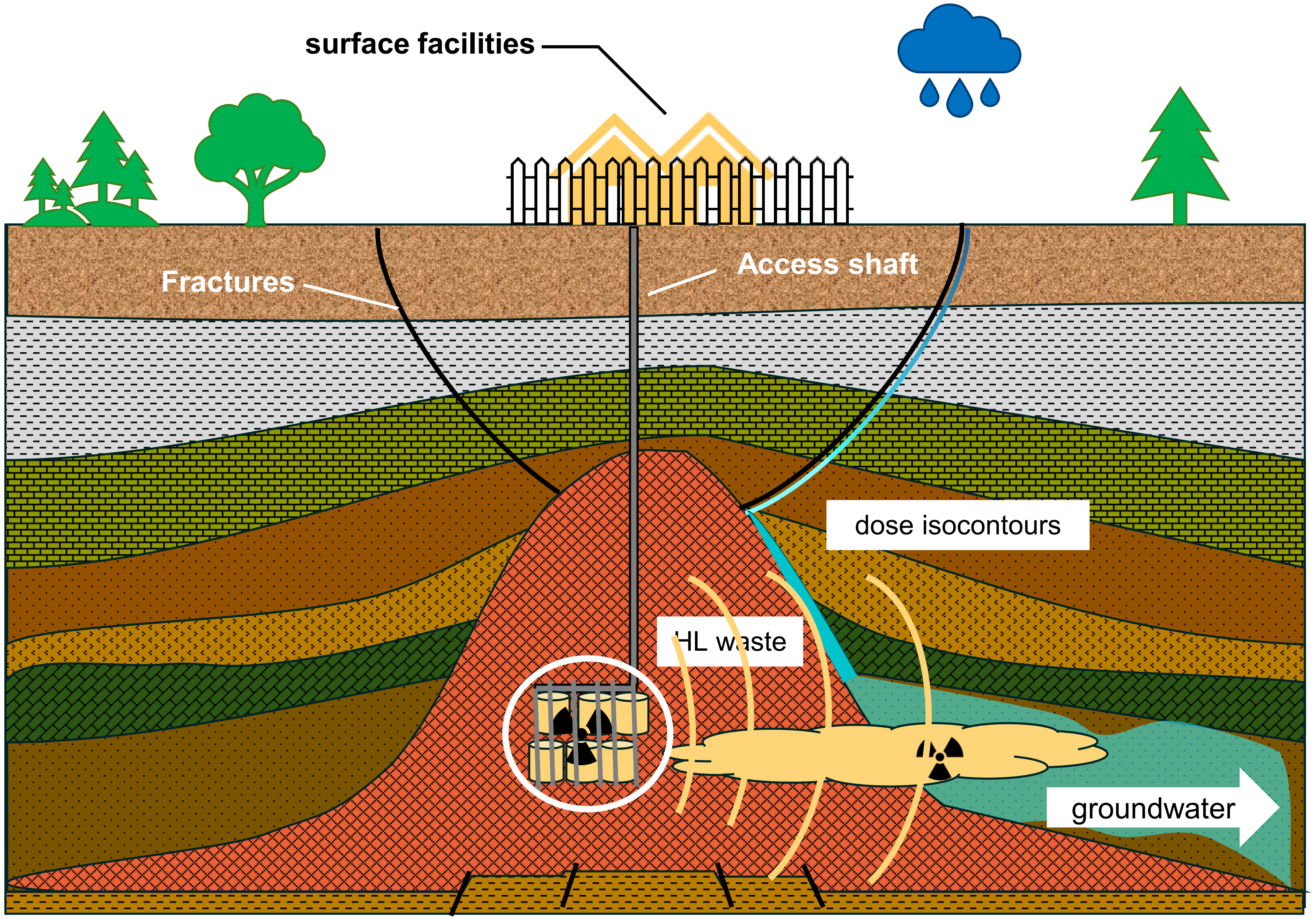
Research objectives



Our knowledge of the subsurface is governed by uncertainties!

Question: How can we disentangle uncertainties, hence manage reliability?

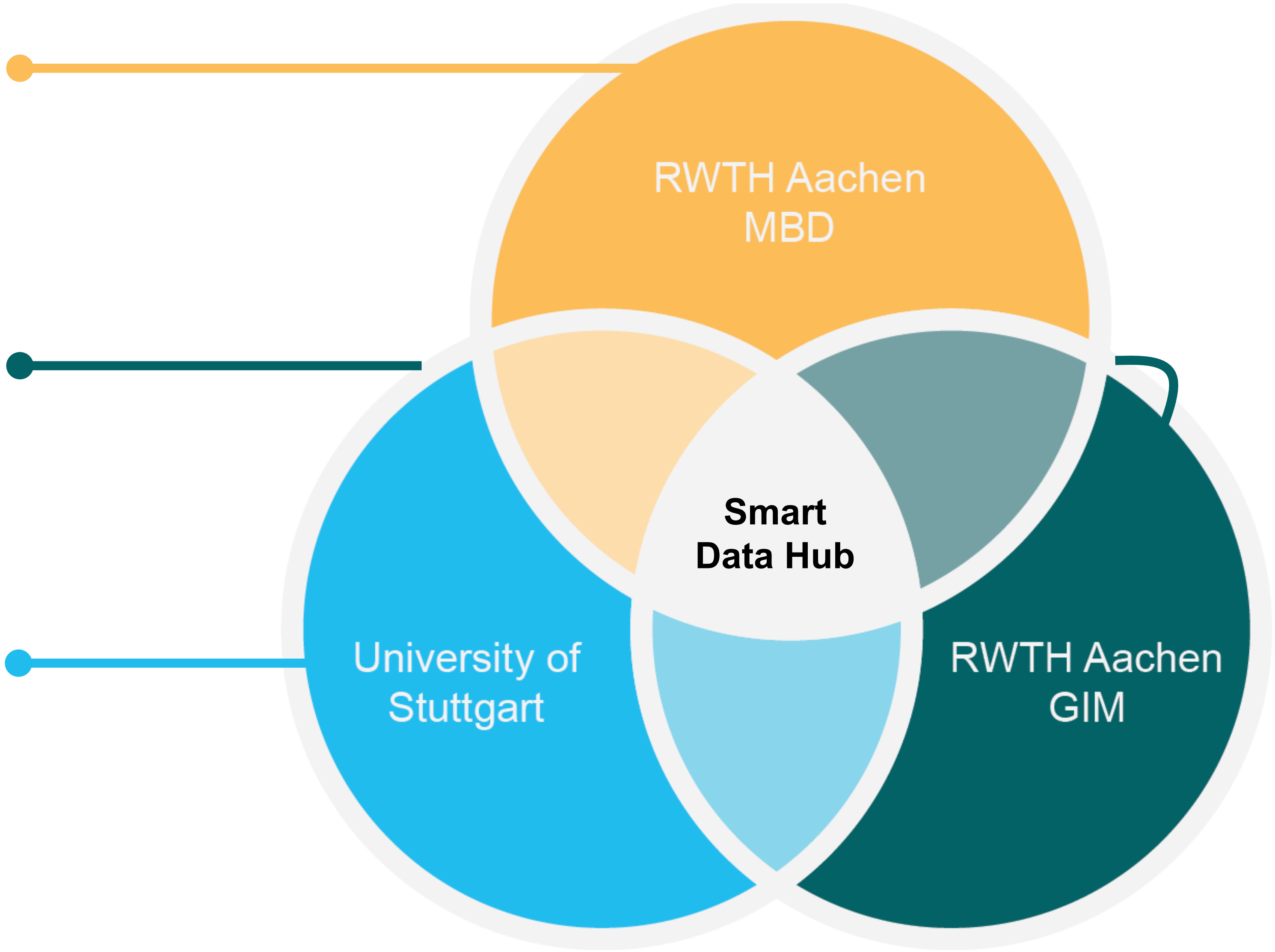
- **Facilitate transparency and reproducibility**
  Collect and integrate system uncertainty; analyze uncertainty impact
- **Decision support for data acquisition (overarching goal)**
  Assess which measurement would be most beneficial to reduce uncertainty
- **Decision support for monitoring radioactive waste repository**
  Assess which measurements would be most beneficial for reliable monitoring

Key methodological building blocks

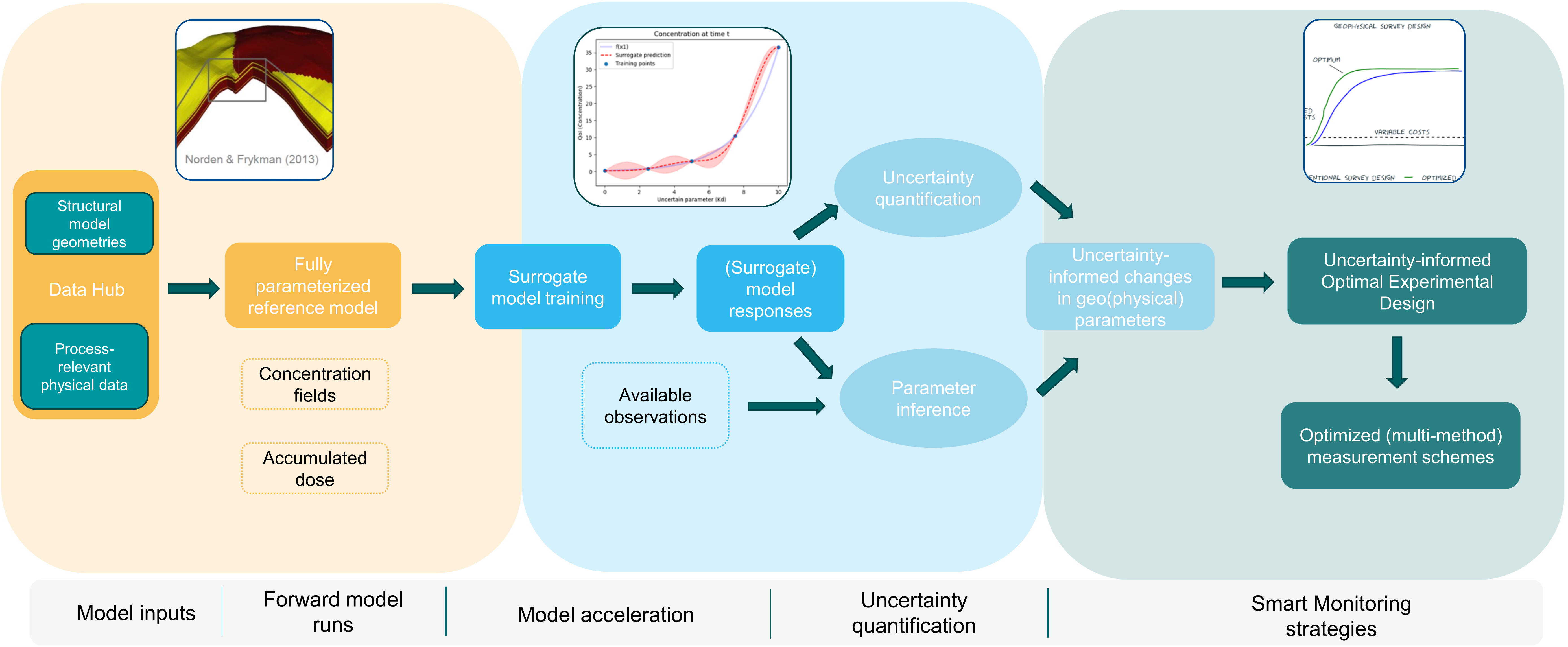
- **Impact modeling**
  orchestrates a workflow based on uncertainty informed geology, hydrothermal setting and impact scenario (nuclide transport)

- **Optimal experimental design**
  uses uncertainty-informed (impact) models to assess the value-add of surface probing and geophysical measurements

- **Surrogate modeling**
  constitutes an enabling technology for compute- intense tasks in impact modeling and optimal experimental design



Framework



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The Need for a Smarter Data Management Tool

We need material properties and uncertainties to feed into our models.

Common challenge: **Data findability**!

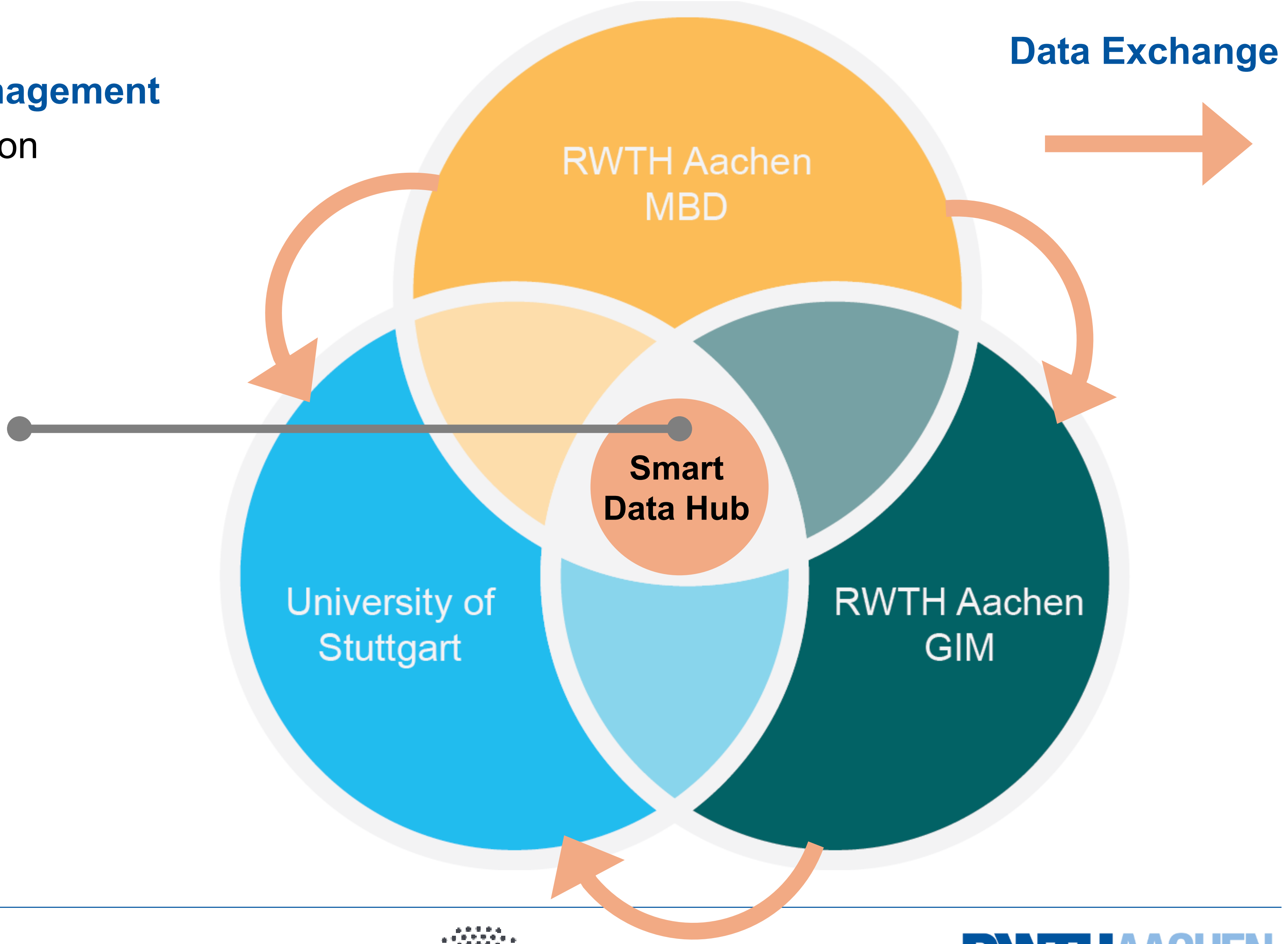
Are we managing it in the most efficient way?

What if we could **seamlessly integrate** this **data into simulation** workflows?

data is structured, **accessible**, and directly compatible with your simulations!

Core digital infrastructure

- **Smart Data Hub**
  A FAIR approach to input/output data management
  idea: provides central instance to collect info on
  - geological site,
  - material properties,
  - subsurface geological model,
  - …



starting point for data-integrated white-box impact model

provides uncertainty information as input for uncertainty management

facilitates traceability and reproducibility

Smart Data Hub: Database

- Rock properties

YAML-DB

density ρ:
- type
- unit
- value/relation
- Uncertainty
- source
- flag

conductivity κ:
- type
- unit
- value/relation
- Uncertainty
- source
- flag

heat capacity c_p:
- type
- unit
- value/relation
- Uncertainty
- source
- flag

porosity φ:
- type
- unit
- value/relation
- Uncertainty
- source
- flag

Sites

synthetic
- DE_Crystalline.yml
- DE_Rocksalt.yml
- ...

reference
- USA_Wipp_Rocksalt.yml
- CH_MontTerri_OpalinusClay.yml

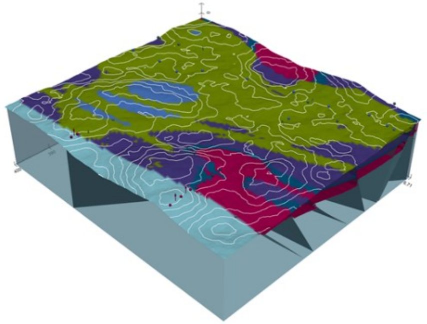
candidate

sensible defaults

age_lithology
- Cenozoic_Claystone.yml
- Cenozoic_Sandstone.yml
- Cenozoic_Limestone.yml
- Mesozoic_Sandstone.yml
- Mesozoic_Claystone.yml
- Mesozoic_Limestone.yml
- Paleozoic_Claystone.yml
- Paleozoic_Sandstone.yml
- Paleozoic_Sandstone.yml
- Paleozoic_Limestone.yml

- Geomodel

GemPy



+ PyVista

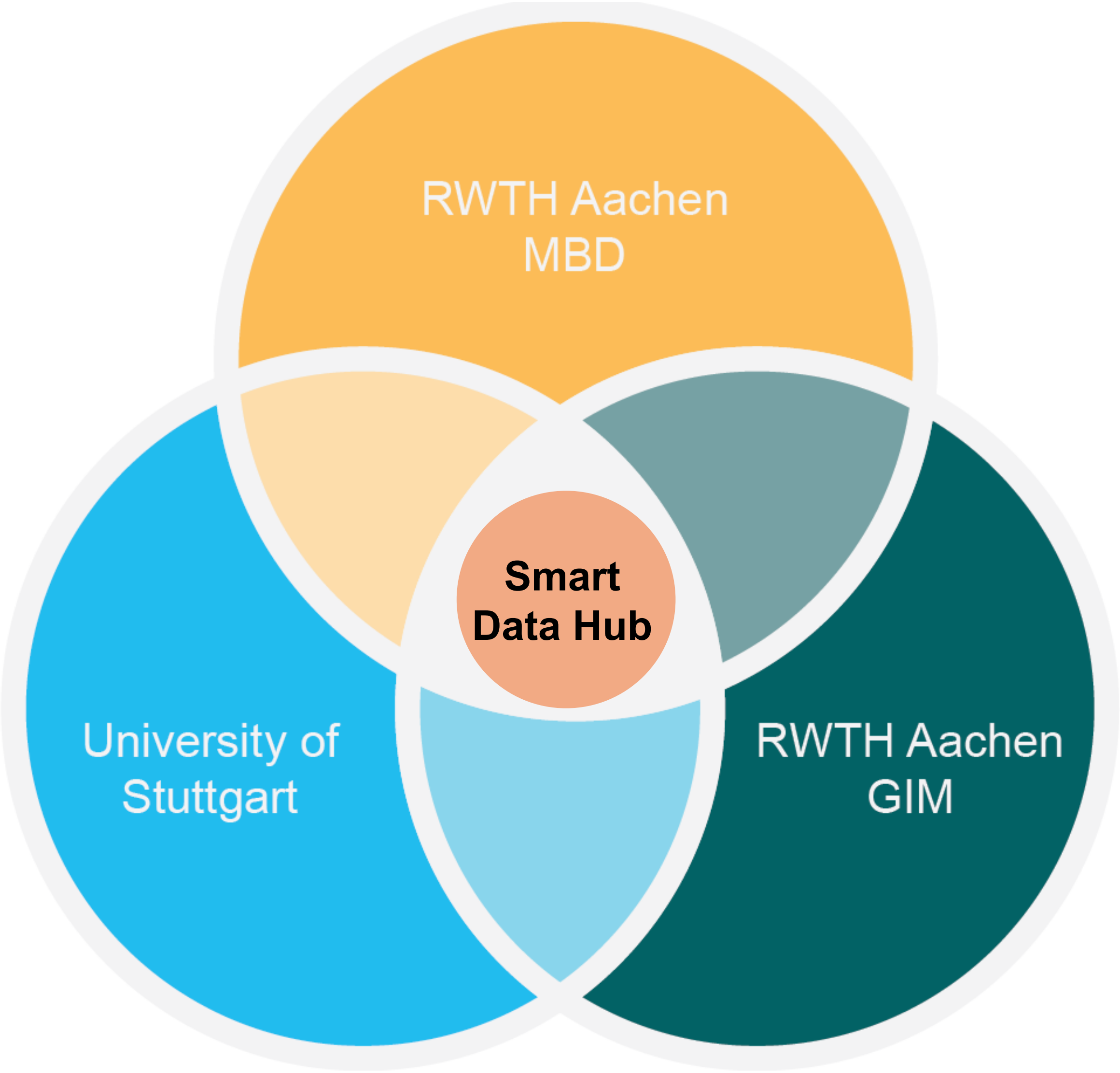
save as plydata for Dashboard visualization

Example:
geometry/USA_Wipp_Rocksalt

- Changhsingian.ply
- Tertiary.ply
- Wuchiapingian-Lower.ply
- Wuchiapingian-Middle.ply
- Wuchiapingian-Upper.ply

Live Demo

Smart Data Hub: Publicly accessible via GitHub



Smart Data Hub - A Data-Centric Approach for Integrated Simulation Workflow Management in Radioactive Waste Disposal

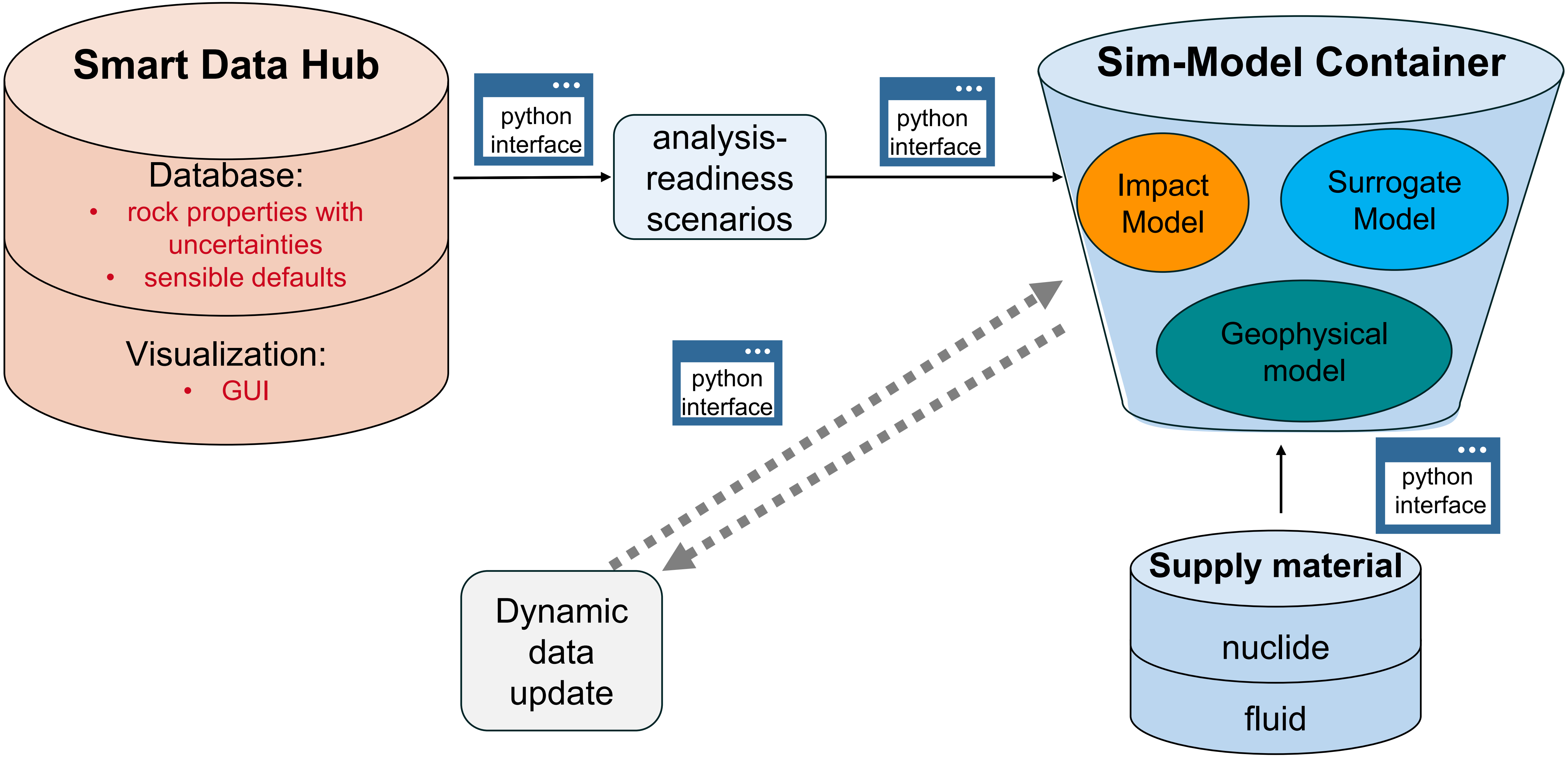
Contribution to a conference proceedings:

- **DECOVALEX 2023, Troyes France**
- **EGU2024, Vienna Austria**
- **Research Data Day2024, Julich Germany**

Available in GitHub

Paper in preparation

Data need to be readily accessible



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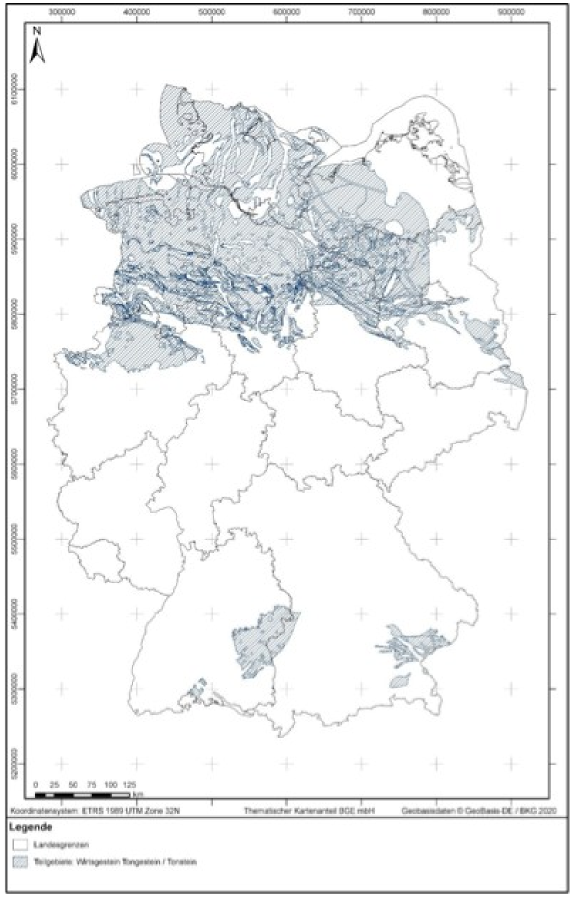
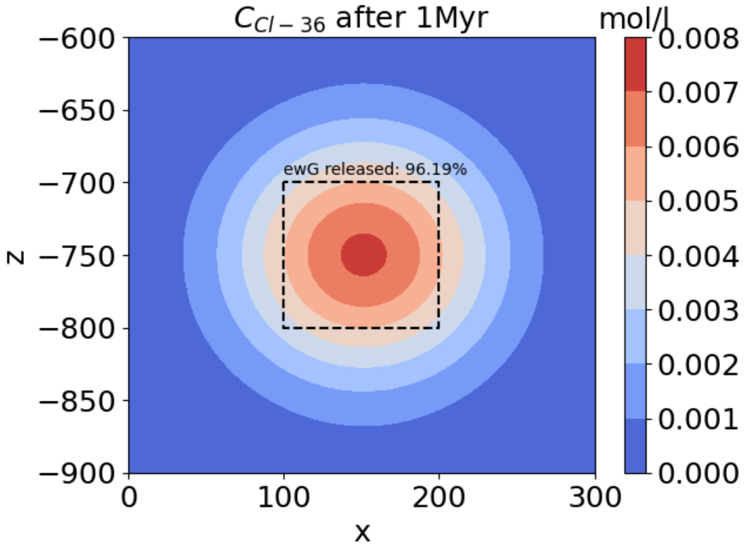
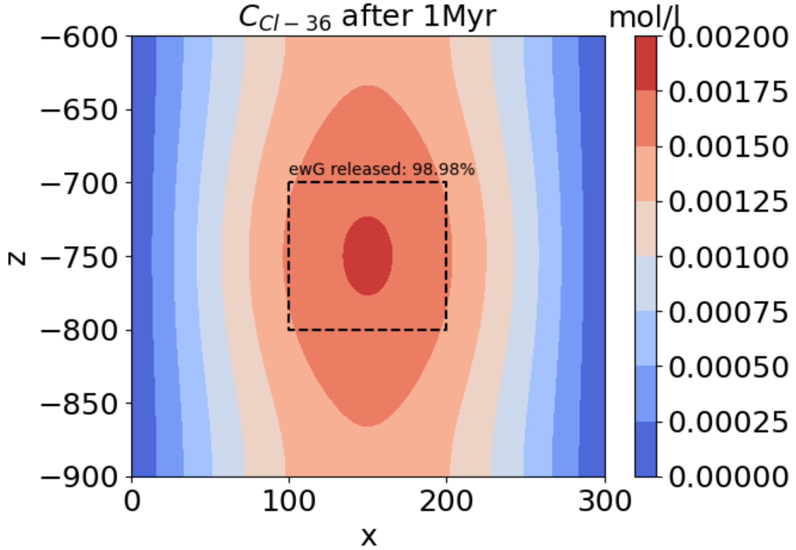
Process and Impact models

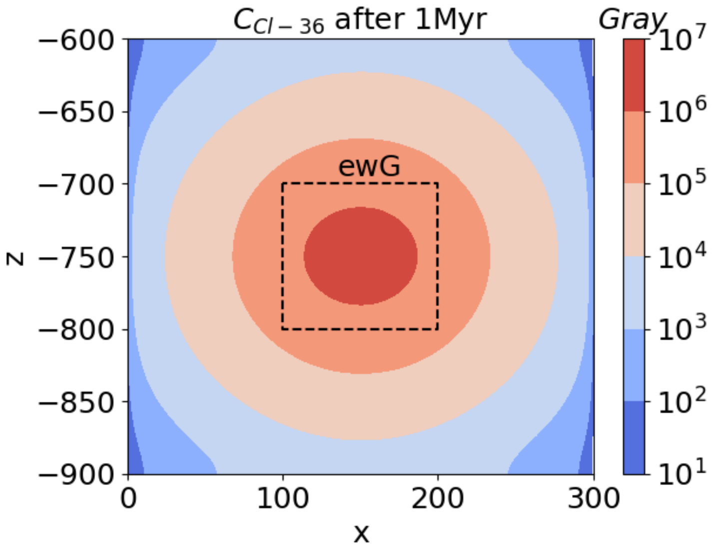
- Claystone

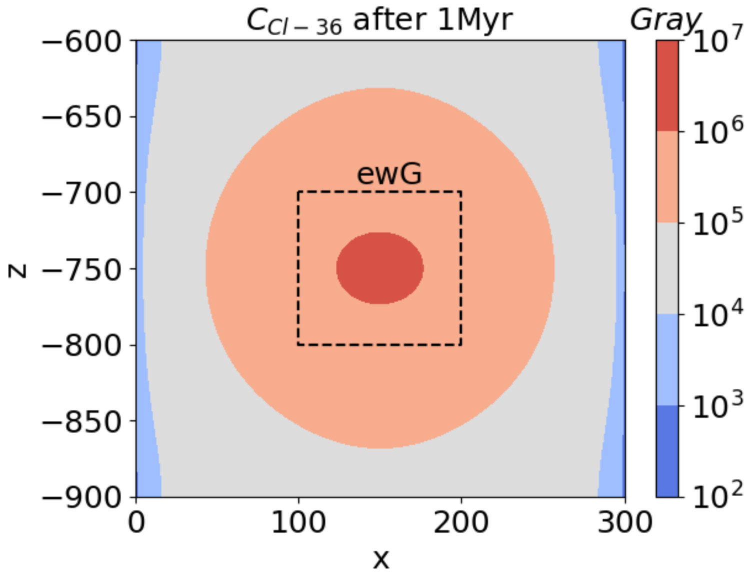


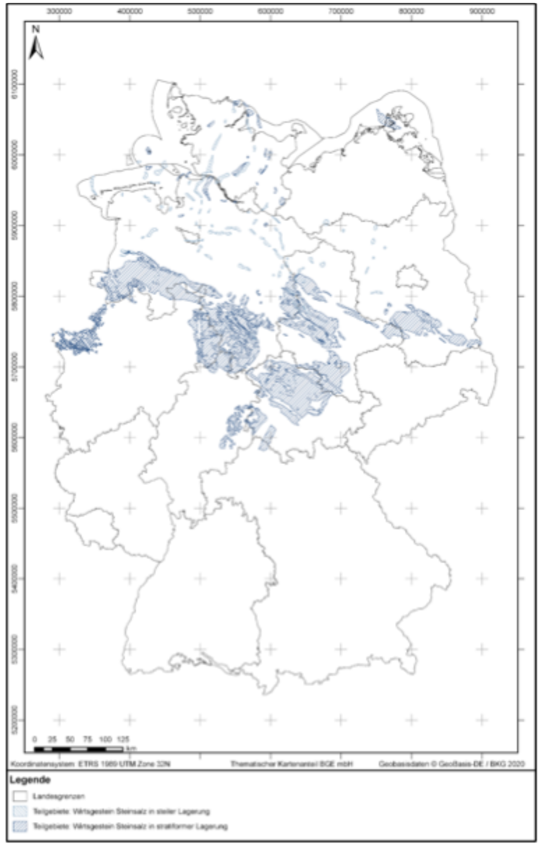




- Rock Salt







Python interface between Smart Data Hub and OGS

Smart Data Hub

send ‘main’ to the Forward Solver

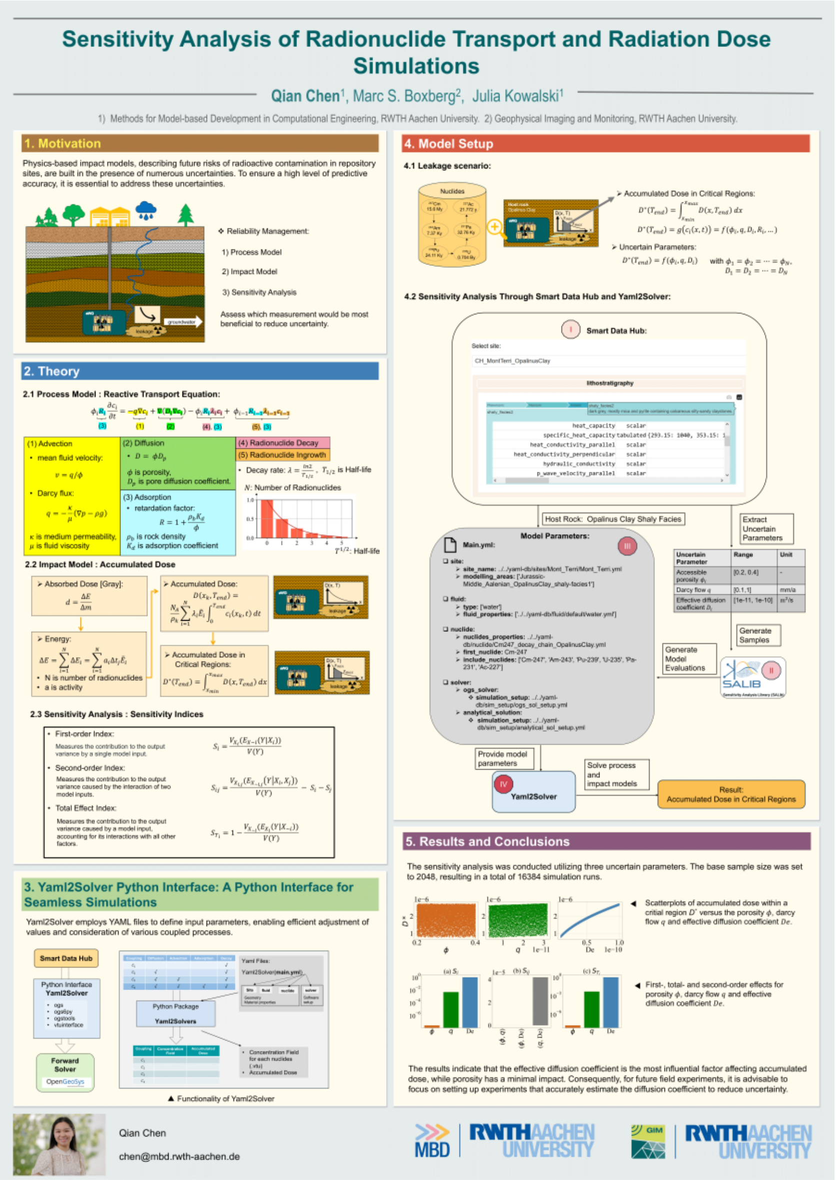
Python Interface
Yaml2Solver

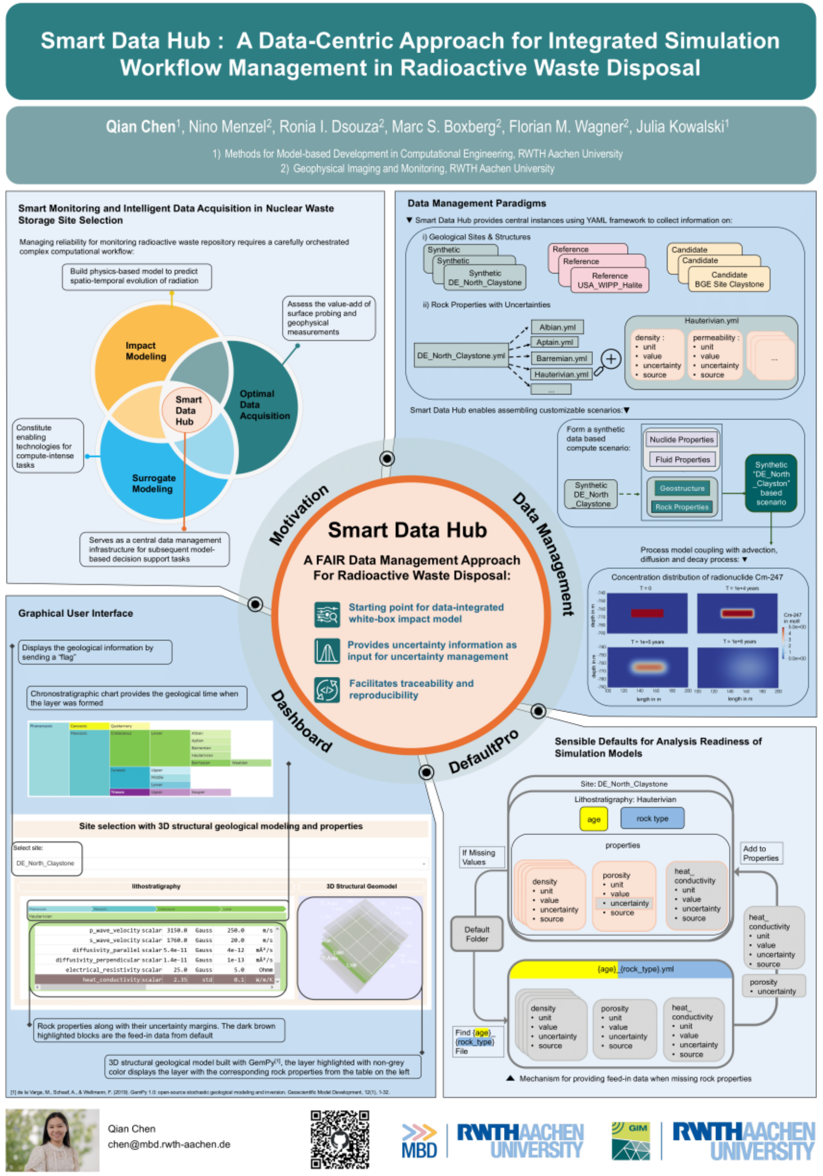
- ogs
- ogs6py
- ogstools
- vtuinterface

Forward Solver

OpenGeoSys
OPEN-SOURCE MULTI-PHYSICS

Poster Session





Surrogate Models in URS

Maria Fernanda Morales, Universität Stuttgart

My main points will be…

- URS needs surrogate models
    - Surrogates have their own uncertainty
- Python package for surrogate model building and UQ
- Surrogates are challenging for models
    - with many parameters
    - with many results

Surrogate Models: What and Why?

Model

Highly detailed geometry & processes uncertain parameters

(Limited) forward model runs

Surrogate

Surrogate model training

What: substitute original models

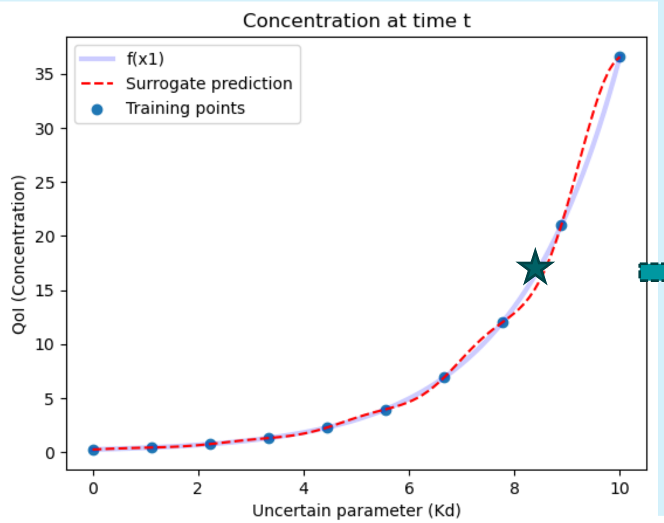
- Trained with few model runs

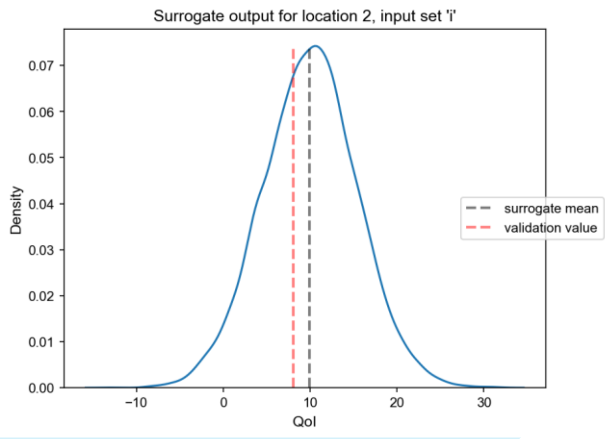
Why: run in a fraction of the time

But: are **approximations**

→ have errors

→ We use surrogates that quantify their uncertainty





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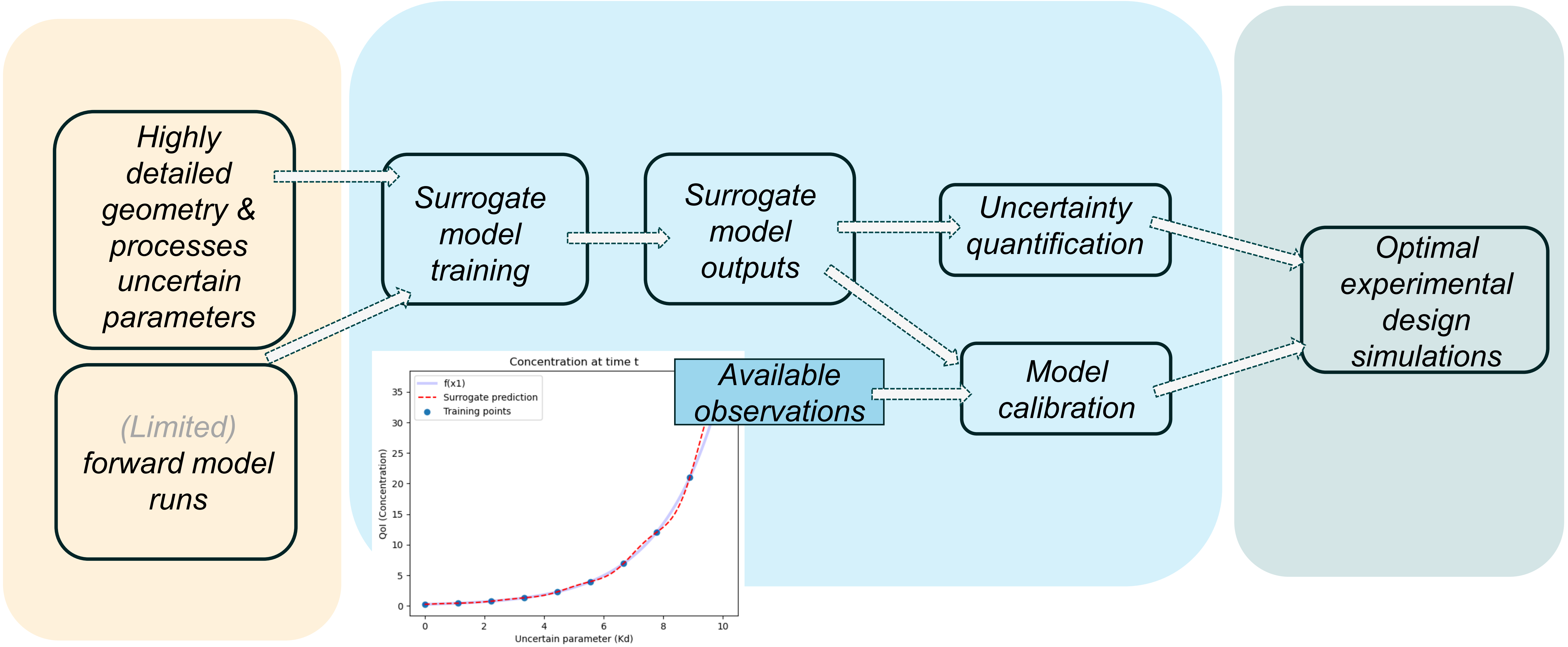
Surrogate Models in Smart Monitoring & URS



Surrogate Model Python Package: BayesValidRox

Easy all-in-one **Bayesian** toolbox for:

- Surrogate model building
  - Optimizes model structure
  - Optimizes selection of original model runs (Active Learning)
- Uncertainty quantification and sensitivity analysis
- Bayesian model calibration
- Model comparison

Available in BayesValidRox 2.0

Website with documentation

In progress

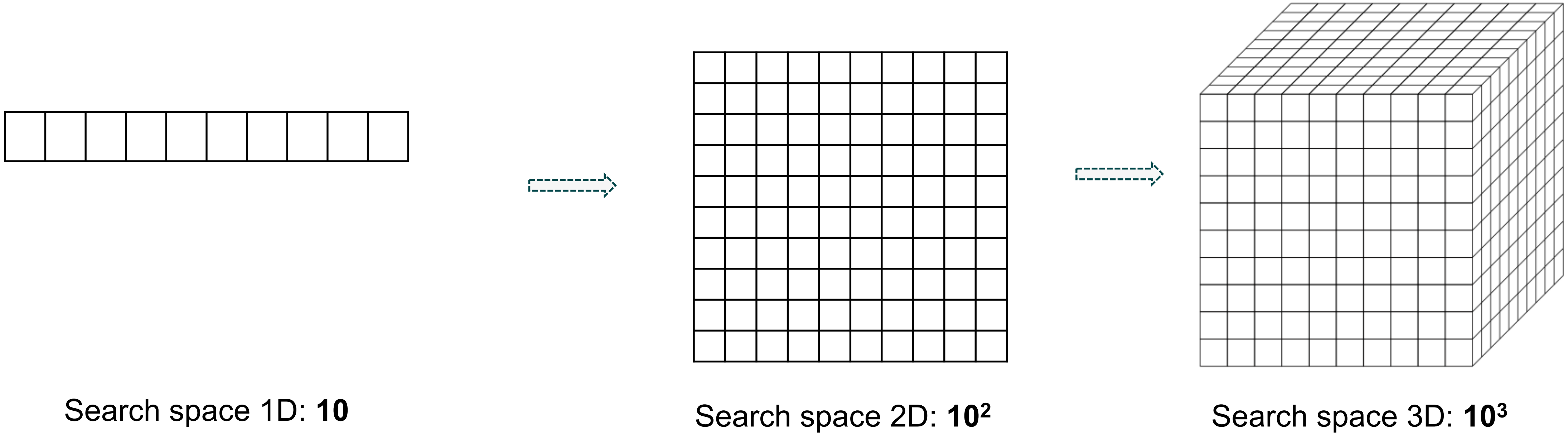
Paper in preparation

https://pypi.org/project/bayesvalidrox/

Phase I | Phase II | Phase III | Post-Closure

What's the problem with "high-dimensional" inputs?

- Surrogate training needs model runs with selected parameter combinations.



- **More parameters are "exponentially bad" (10, 100, 1000 parameters?)**
- **Our approach**: Input dimension reduction for surrogate training
  - There is an error associated to it, which we must consider during training and use of the surrogate

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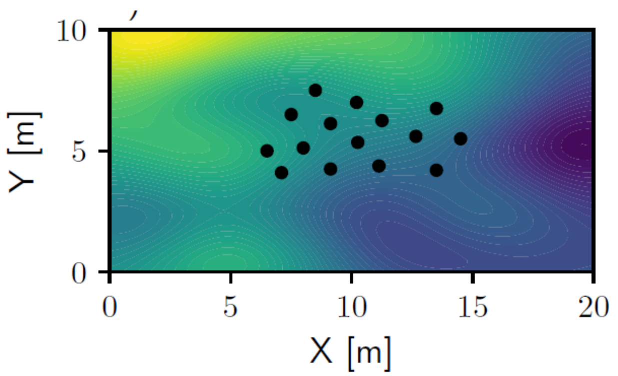
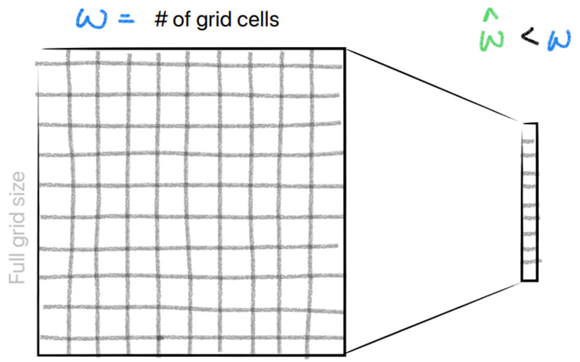
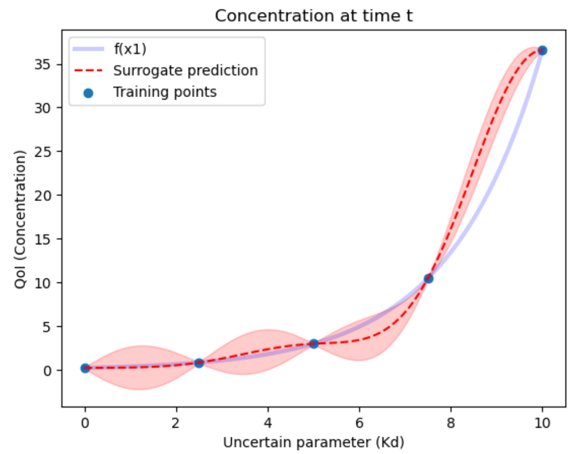
To the rescue: “input dimension reduction”

High dimensional problem → Input dimension reduction (IDR) approach → Surrogate training on reduced inputs





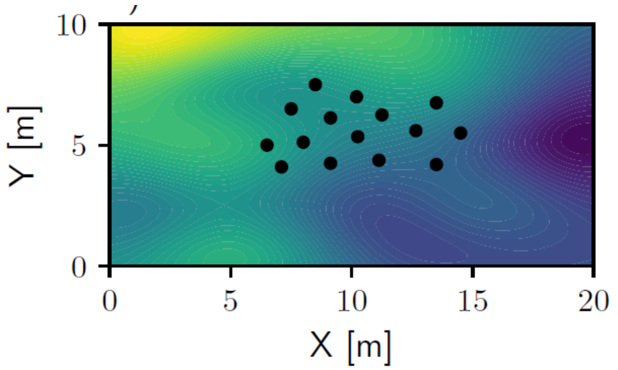


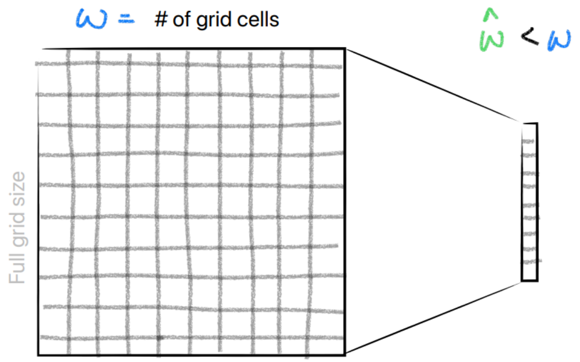
Goal: Find a **smaller** combination of parameters that represent most of the original parameter variability

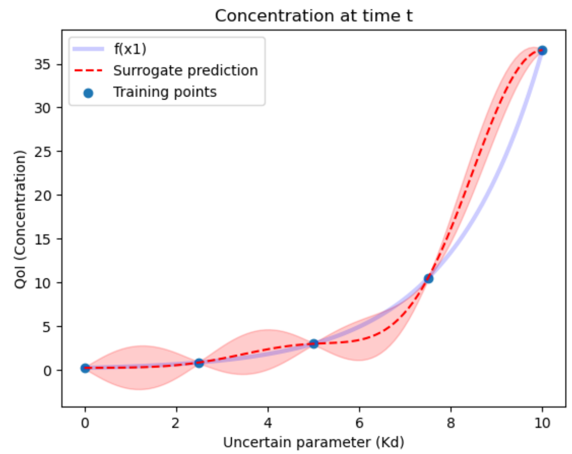
- Examples: PCA, SVD as in PEST, VAE
  - Makes surrogate building cheaper
- Quantify the uncertainty through input reduction together with all other uncertainties → **see our poster**

To the rescue: “input dimension reduction”

High dimensional problem → Input dimension reduction (IDR) approach → Surrogate training on reduced inputs







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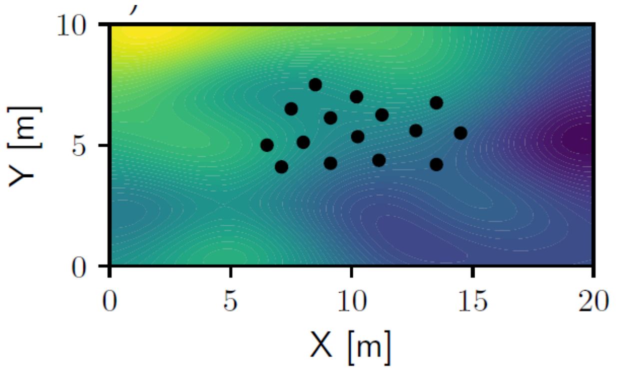
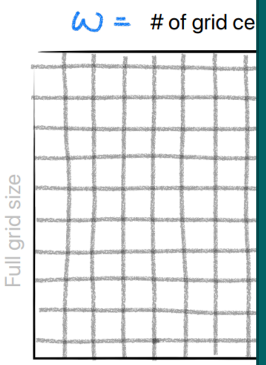
To the rescue: "input dimension reduction"

High dimensional problem → Input dimension reducti… app…

Surrogate training…





Methodologies presented in EGU2024[1] and GeoEnv2024[2] conferences and 1 paper publication[1]

Paper and technical note in preparation

[1] **Morales Oreamuno MF**, Oladyshkin S, Nowak W. Error-aware surrogate modelling with input dimension reduction for groundwater modelling in heterogeneous media. In: Geophys Res Abstr. Vienna: EGU General Assembly 2024; (Geophys. Res. Abstr.; Bde. 26, EGU24-12586).

[2] **Morales Oreamuno MF**, Oladyshkin S, Nowak W. Training surrogate models using input dimension reduction and Bayesian active learning techniques for inverse modelling in heterogeneous media applications. In: geoENV2024 Book of Abstracts. Chania, Crete, GR:; 2024. S. 191--192. (geoENV2024 Book of Abstracts).

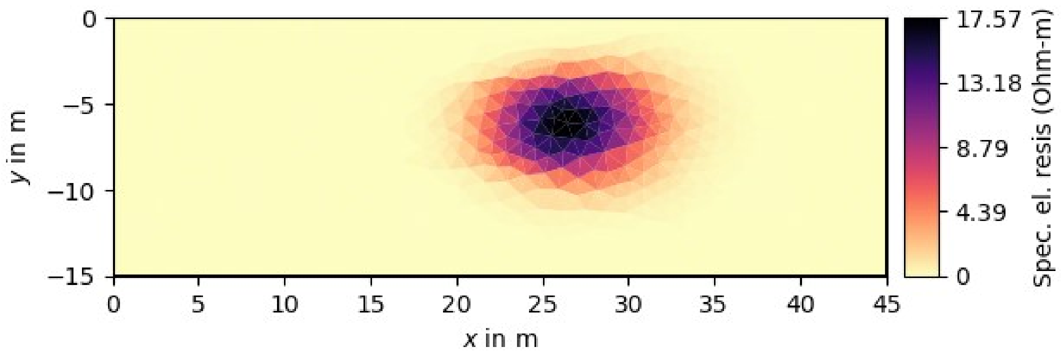
[3] Kröker I, Brünnette T, Wildt N, **Oreamuno MFM**, Kohlhaas R, Oladyshkin S, u. a. Bayesian3 Active Learning for Regularized Multi-Resolution Arbitrary Polynomial Chaos using Information Theory. International Journal for Uncertainty Quantification. September 2024;

Goal: Find a **smaller** combination of p…

- Examples: PCA, SVD as in PEST, VAE
  - Makes surrogate building cheaper
- Quantify the uncertainty through input reduction together with all other uncertainties → **see our poster**

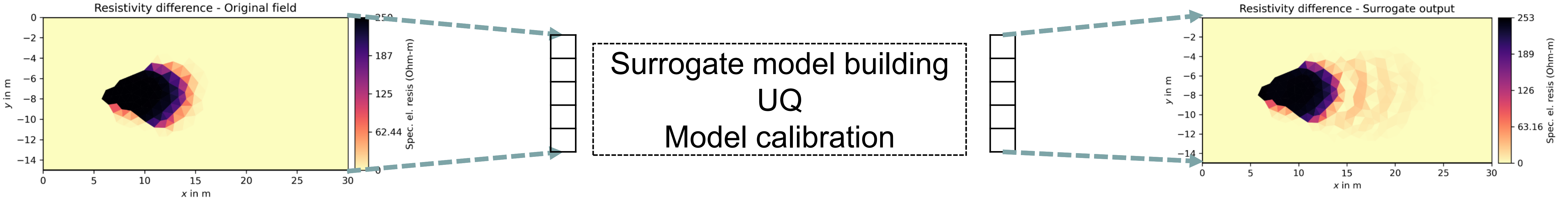
What's the problem with "high-dimensional" OUTPUTS?

- When we have outputs on a 2D/3D grid and over time → large number of outputs



- Potential problems:
  - Each output/cell = 1 individual surrogate
  - Computationally expensive to train and to evaluate
- For **optimal experimental design** you need the space/time resolution

To the rescue: "OUTPUT dimension reduction"



1. ZIP your problem

2. Do everything on ZIP level

3. Un-ZIP your problem

- **Goal**: smaller representation of our outputs (like a ZIP file):
  - Example: PCA, SVG, VAE
- Accelerate OED simulations
- **See our joint poster**

Work in progress

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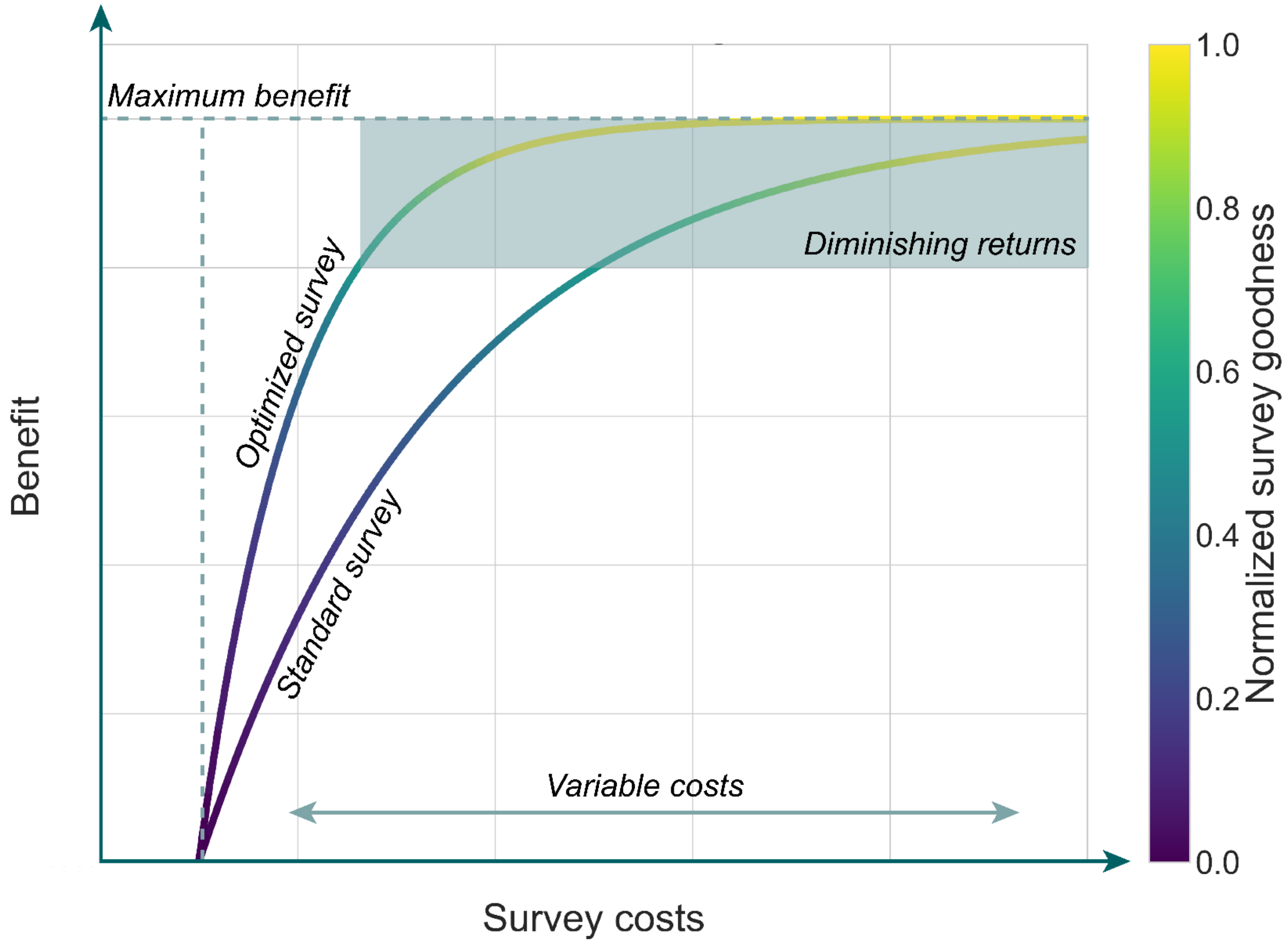
Nino Menzel, GIM, RWTH Aachen

My main points will be…

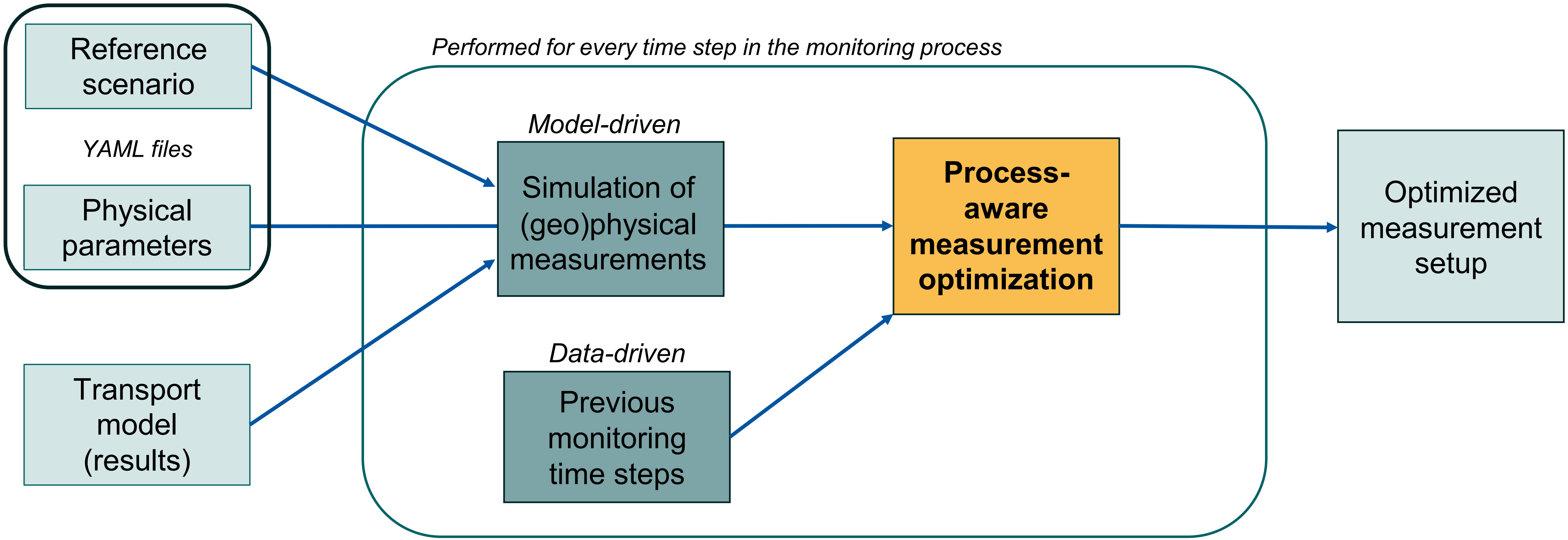
- URS needs smart monitoring strategies
- We use process-aware optimization strategies
- Survey optimization strategies are applicable to
  - surface exploration
  - subsurface exploration and process transport monitoring

Smart Data Acquisition – Overall Concept



- "**Smart**" data acquisition aims at reaching the point of **maximum benefit as fast as possible**
- **Benefit** of a survey: resulting **net increase in resolution** of model parameters of interest
- Overall goal: **limit** the amount of acquired data (and **variable survey cost**) without drastically reducing information content
- In our case: **effective monitoring of fluid transport processes** using (geo-)physical surveys

Smart Data Acquisition – Workflow



Input from ***DataHub*** | *Modelling in* ***pyGIMLi & OED software package*** *(in preparation at GIM)* | *Output to* ***DataHub***

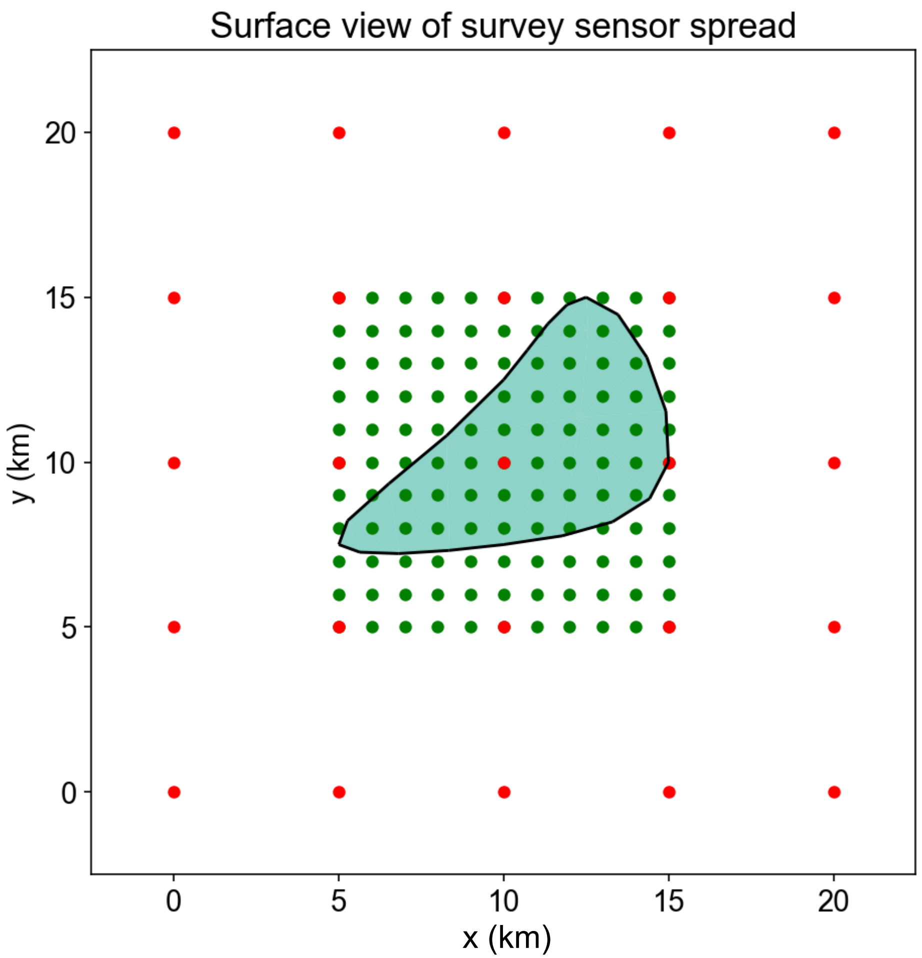
Smart Data Acquisition – Methodology

Inputs:

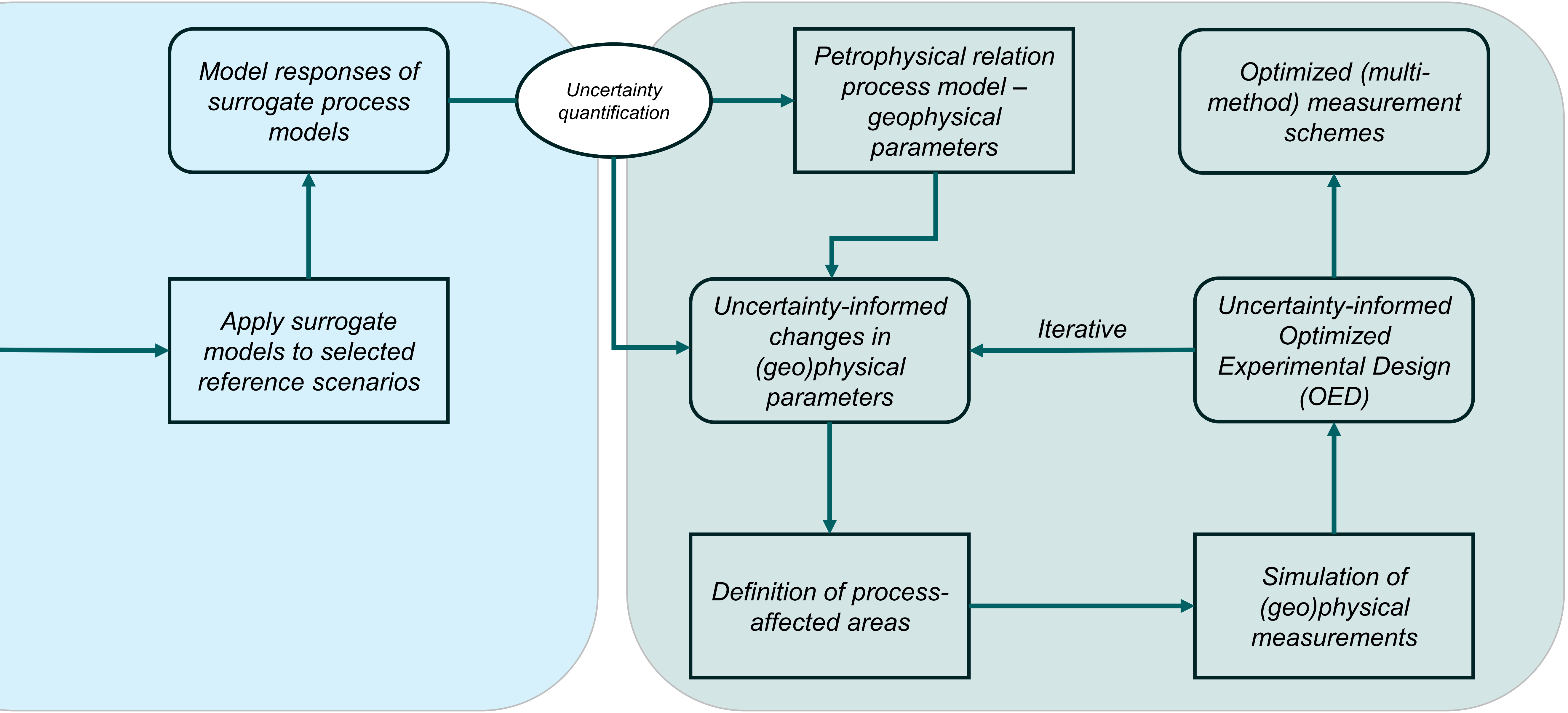
- **A-priori information** of the **target area** in the subsurface (transport process: *hydr. parameters*; geological structure: *geometrical parameters*)

- "Small" **base measurement** setup
  - Seismic tomography survey with *40* receivers and *5* shot points
  - Geoelectric survey using *20* electrodes

- **Densest** possible **measurement setup** (*comprehensive dataset*)
  - Seismic tomography survey with *n* receivers and *m* shot points
  - Geoelectric survey with *n* electrodes



Smart Data Acquisition – Optimization Strategy



Phase I Phase II Phase III Post-Closure

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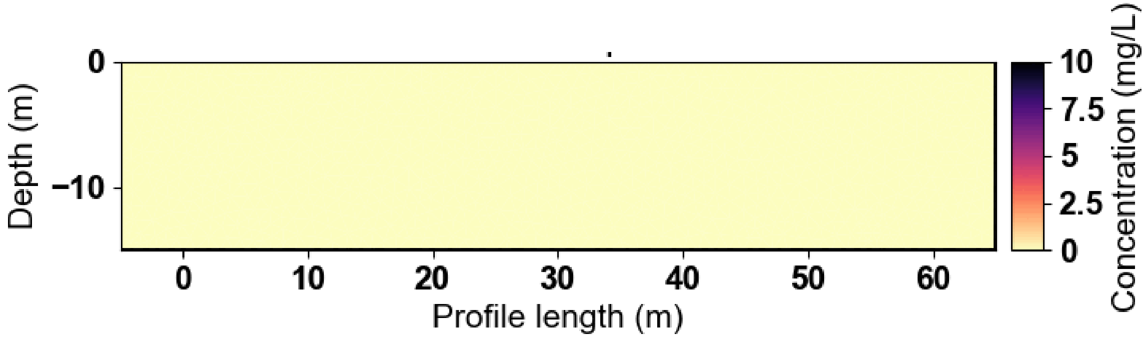
Smart Data Acquisition – Transport Process Monitoring Example

- Optimization algorithms **consider underlying transport process**
- **Focusing** of data acquisition on area that is affected by transport process
- Include **parameter uncertainties** in focusing
  - Multiple model runs with **different physical parameter sets**
  - Consider uncertainties **during optimization**
- Utilize both model predictions and inverse model of acquired data to evaluate simulation quality and **adjust underlying transport model** if necessary



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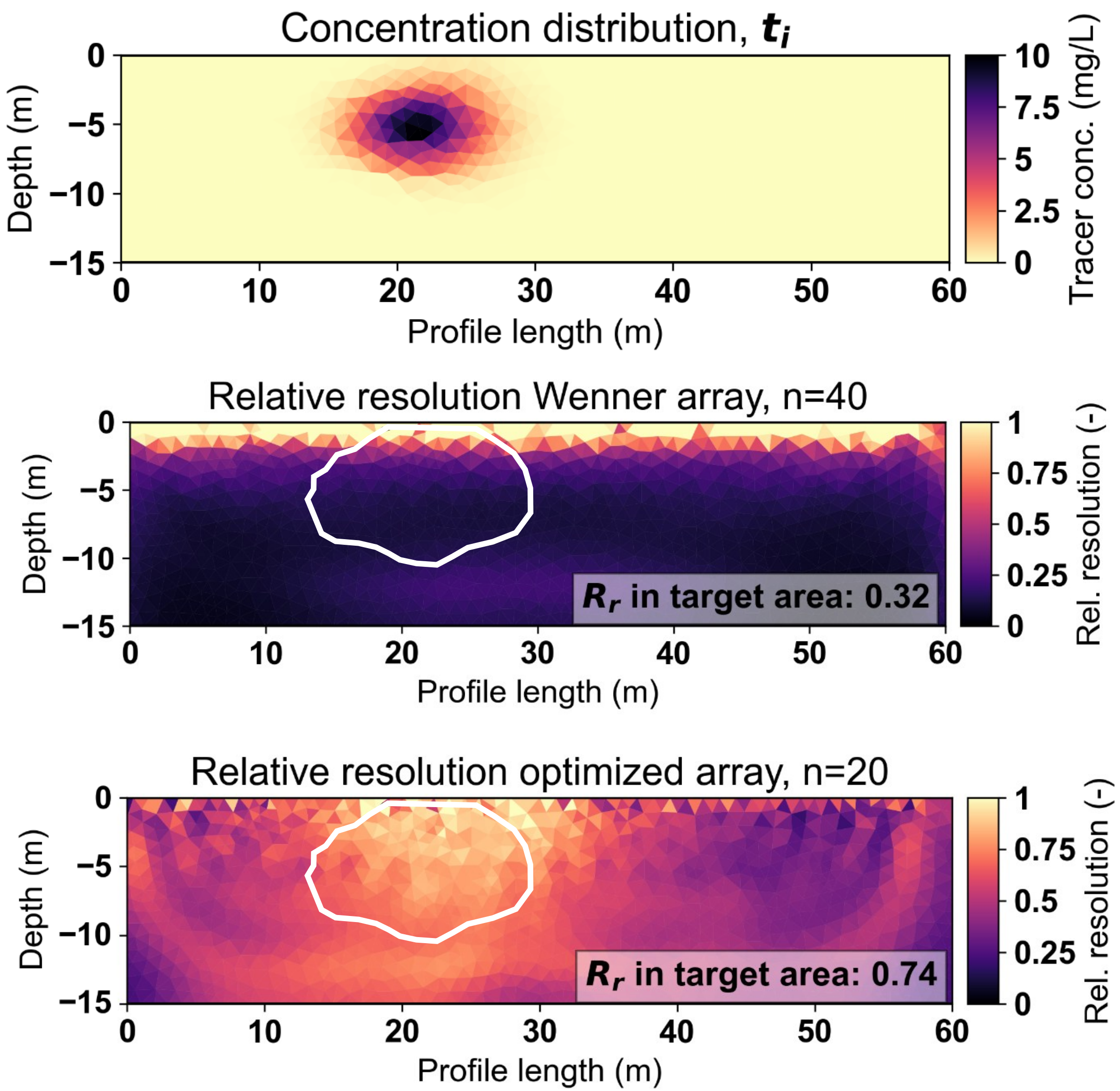
- Process information can come from **any transport simulator and/or real-time monitoring data**



Phase I Phase II Phase III Post-Closure

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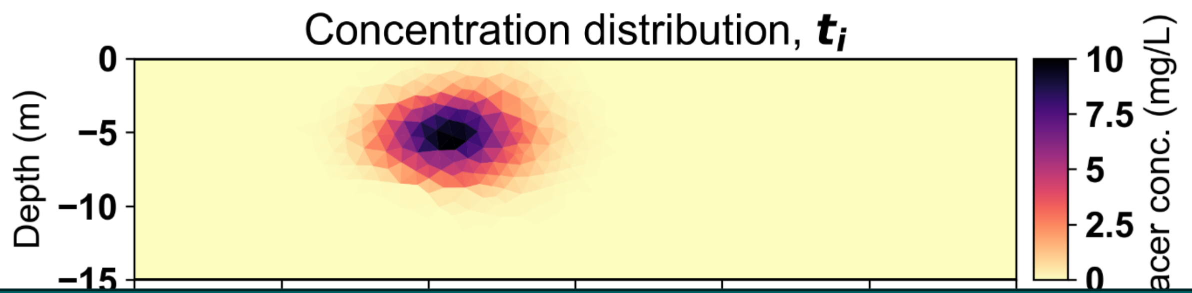
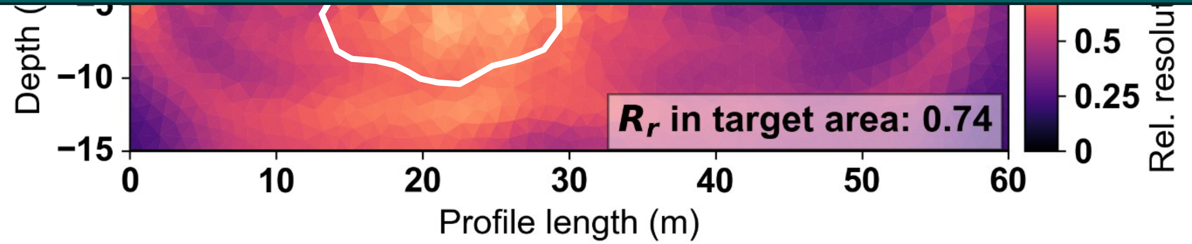


Menzel, N. and Uhlemann, S. and Wagner, F. M. (2024): Strategies for geoelectrical monitoring of subsurface fluid transport processes using Optimized Experimental Design.

EGU General Assembly, Vienna, 14-19 April 2024.

84. Jahrestagung der Deutschen Geophysikalischen Gesellschaft, 10.-14. März, Jena.

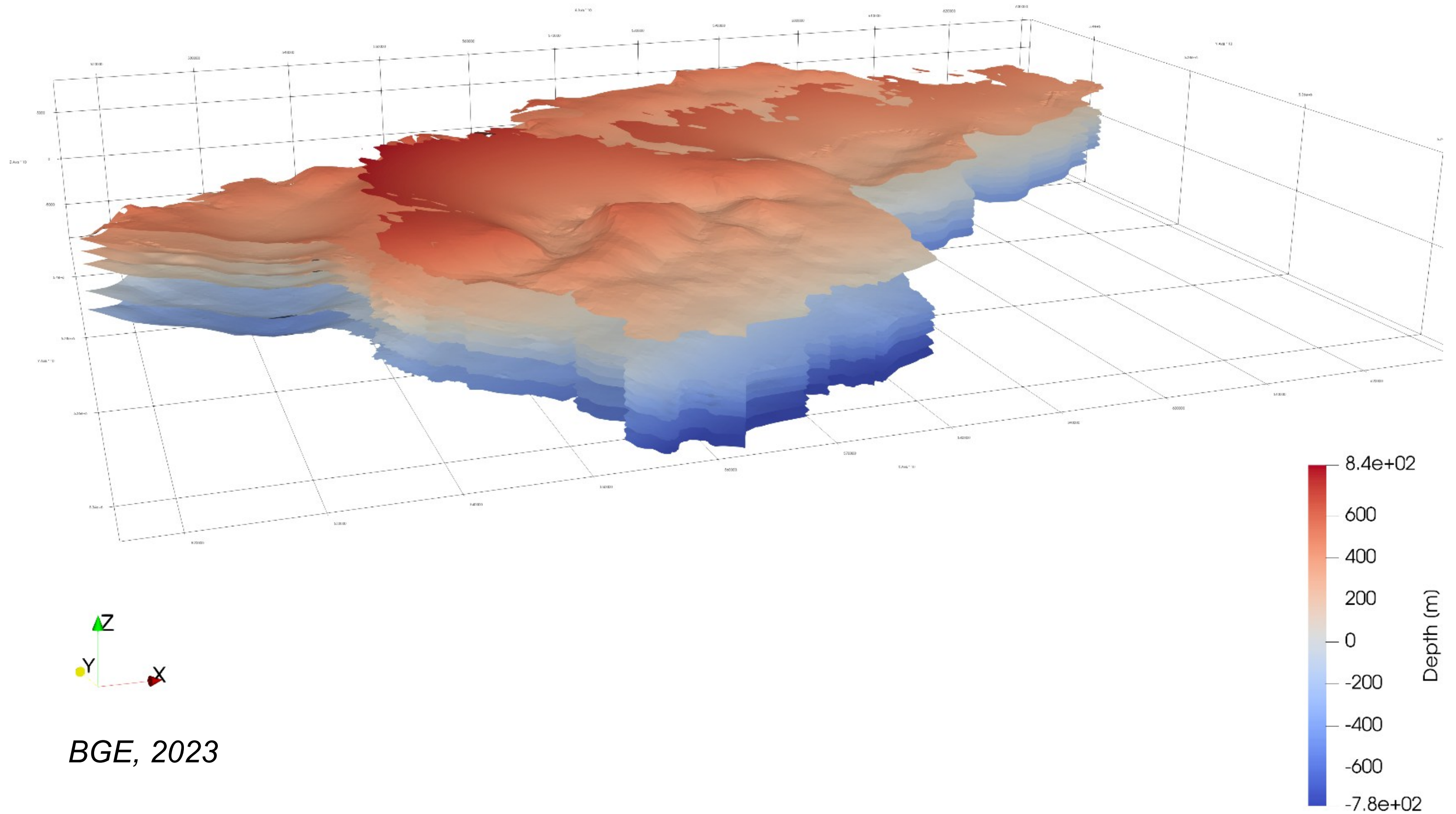
Paper in internal review



Smart Data Acquisition – OED for Site Exploration

OED can also be applied to focus surveys on **static targets**, e.g. **geological features**

- Optimize positions of sensors for surface or borehole exploration
- Optimize length and orientation of geophysical surface and borehole surveys
- Goal: **increase coverage** of measurements **in targeted area**



BGE, 2023

Key Takeaways

Key takeaways:

- **Smart Data Hub** provides **analysis-ready data with uncertainties** that **seamlessly integrate with simulation workflows**
- **Surrogate models enable uncertainty quantification** for computationally expensive models
- Method-agnostic and process-aware “Smart monitoring” strategies are **key for resource-efficient and reliable data acquisition.**
- Surrogates enable **uncertainty-aware OED methodologies**, which require a large number of model runs

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Thank you for your attention!

Smart Data Hub
chen@mbd.rwth-aachen.de

BayesValidRox
maria.morales@iws.uni-stuttgart.de

SmartDOT
nino.menzel@gim.rwth-aachen.de