



The site selection data hub: a data-centric approach for integrated simulation workflow management in radioactive waste disposal site selection

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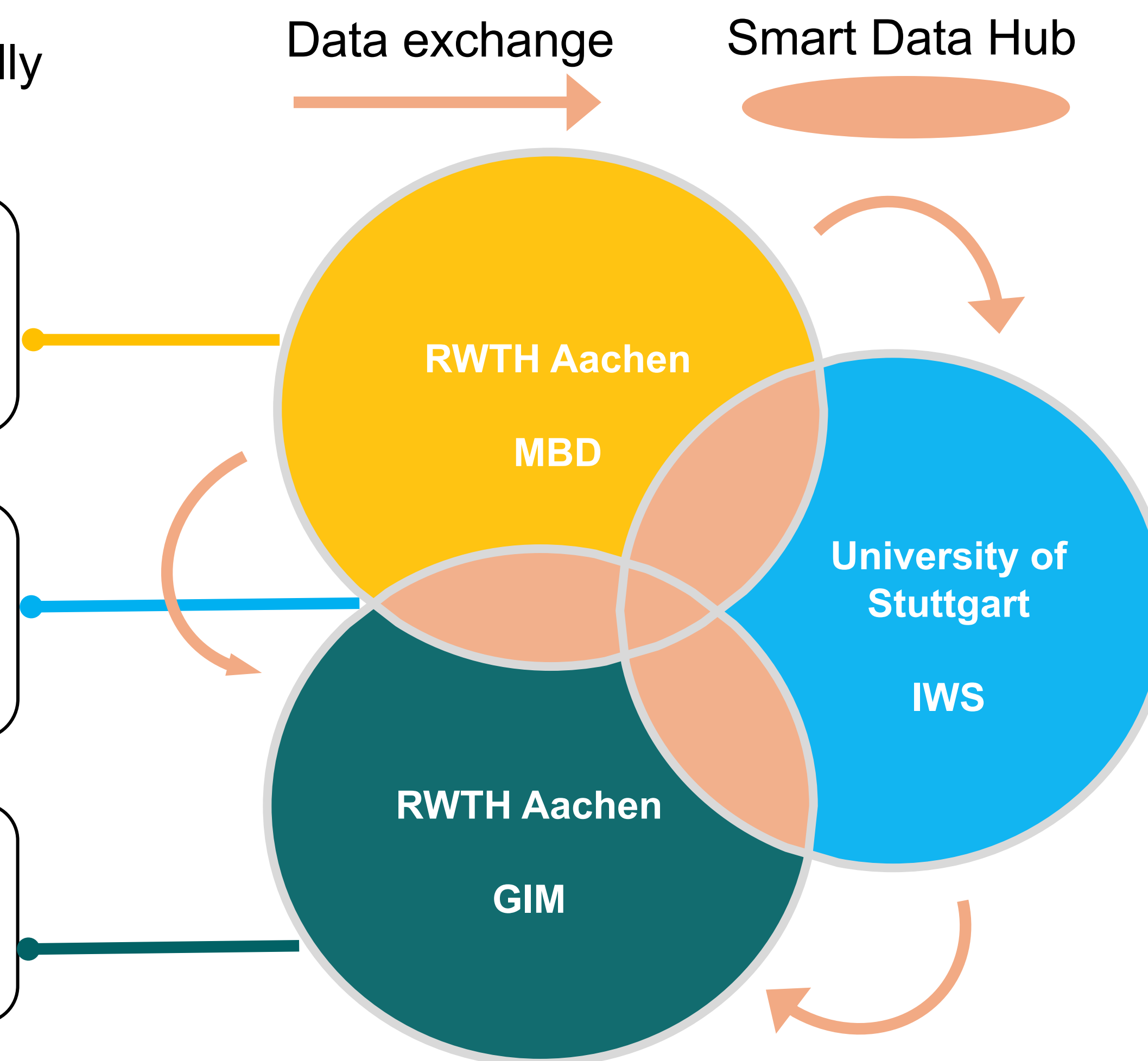
Motivation: Smart Monitoring and Intelligent Data Acquisition in Nuclear Waste Storage Site Selection

Assessing the value-add of data management requires a carefully orchestrated complex computational workflow:

1. Developing benchmark scenarios and projecting the impact scenario into uncertainty-informed hazard maps.

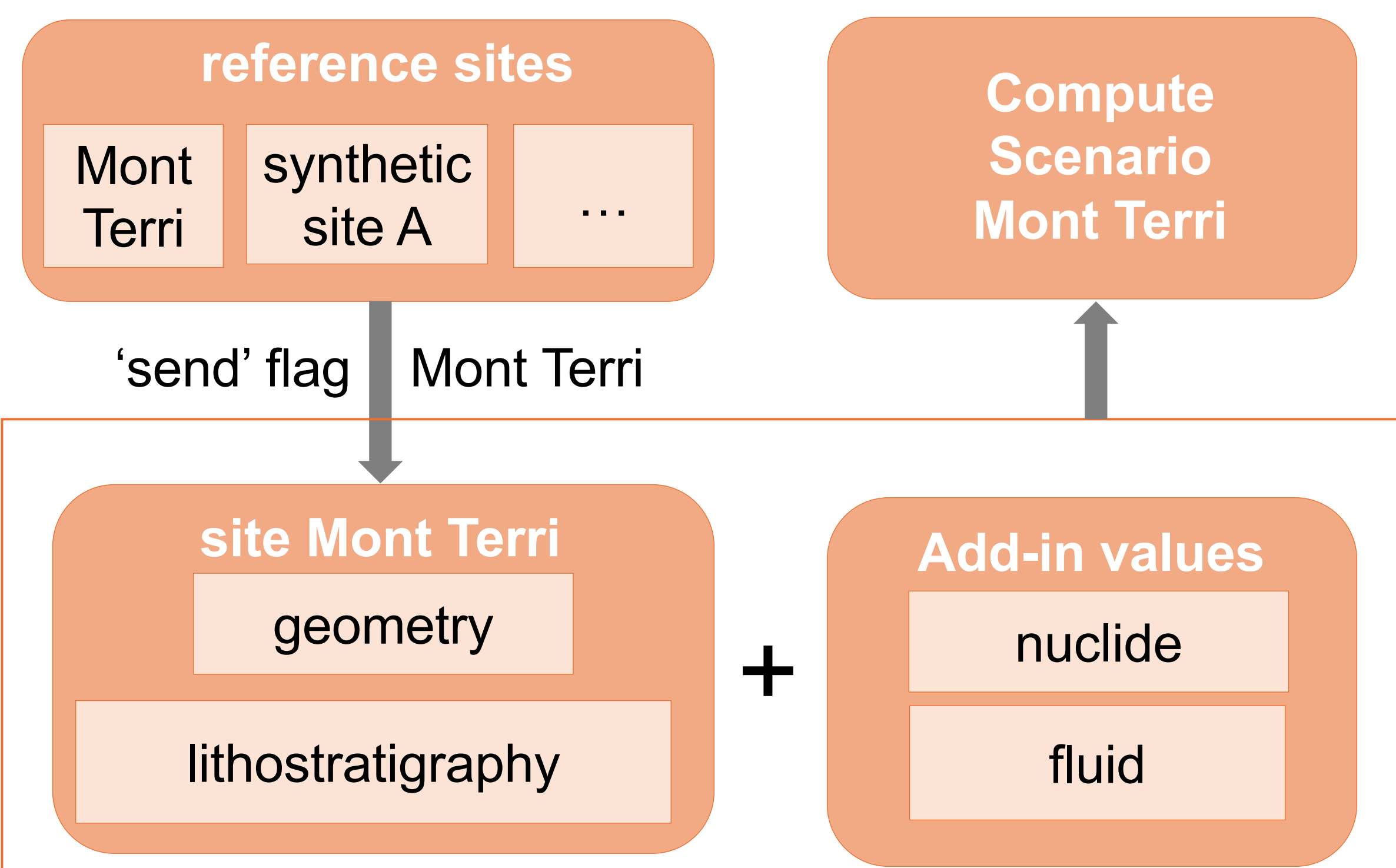
2. Constituting an enabling technology, i.e., a surrogate model for compute-intensive tasks in impact modelling and to quantify the uncertainty.

3. Implementing smart data acquisition to plan surface probing and geophysical measurements.



Smart Data Hub

We established a data-centric approach built with Python. The Smart Data Hub provides simulations with direct access to a database of essential material properties, their associated uncertainty margins and meta information constructed with YAML format.



This Smart Data Hub serves as the central management system for our project. It facilitates:

- Uncertainty-informed scenario-based simulations.
- Training in surrogate.
- Assessing data acquisition strategies.

Scenario-based Simulations: Process & Impact models

The input parameters for the simulation are provided by the compute scenario generated from Mont Terri flag properties.

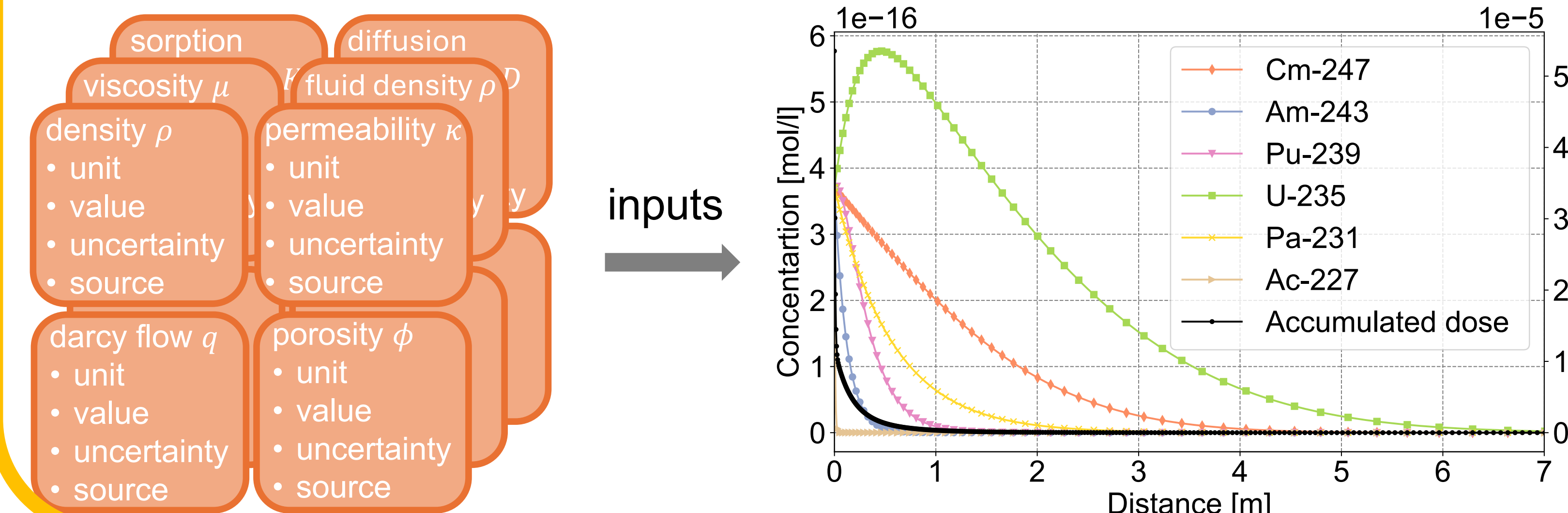


Figure 2: The concentration evolution of the simplified Actinium decay chain and the accumulated dose after 1 million years utilizing input parameters obtained from measurements conducted at the Mont Terri rock laboratory.

Surrogate Strategy

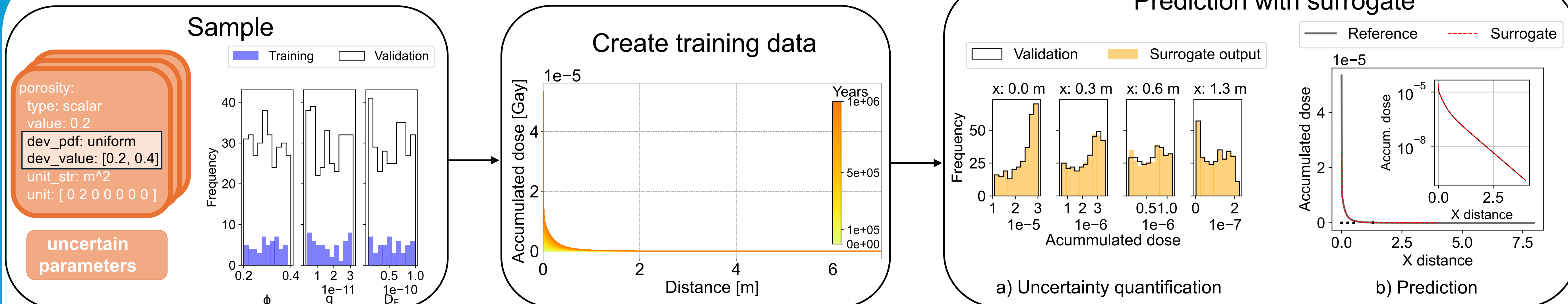


Figure 3: Training samples can be obtained using the information in the Smart Data Hub and evaluated in the forward model. The surrogate is then trained and can be used for uncertainty quantification and/or prediction for computationally expensive models.

Smart data acquisition

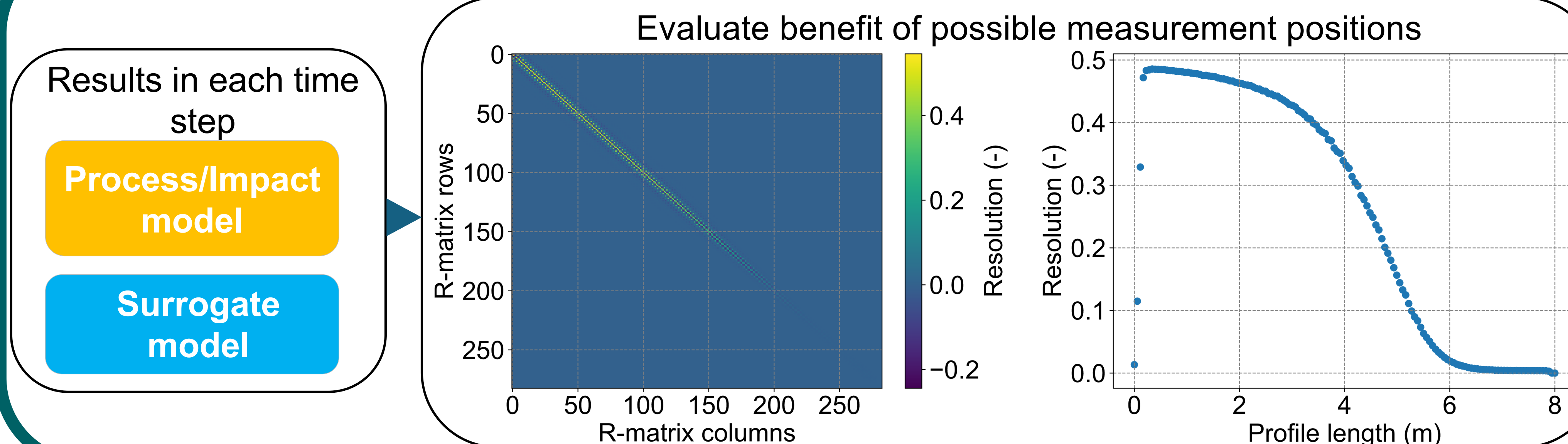


Figure 4: (Geo)physical measurement setups are optimized by calculating the increase in resolution that would be achieved by placing sensors at different positions along the nuclide transport path. Therefore, a reference set (set of the densest measurement setup possible) is utilized to choose candidates from.

Conclusion

Our study introduces the Smart Data Hub, a data-centric management infrastructure for executing modular workflows. It enhances information interchangeability across workflow stages, facilitates scenario-based integrated simulation with uncertainty, as well as demonstrates the feasibility of conducting transparent, reproducible, and uncertainty-informed studies.

Figure 1: The data structure is configured in a scenario-based framework, where a compute scenario is constituted by the material properties of a specific site combined with desired add-in values. Material properties linked to the particular sites are accessible via designated flags associated with the sites.