Technische Universität Braunschweig

Optimization enabled digital twinning of radioactive waste repositories

Henning Wessels, 21.09.2022

My Way to IGD-TP

Roadmap on Artificial Intelligence in radioactive waste disposal

Krafcyzk et al., 2021

Involved parties: BGE Tec, GRS, Helmholtz, TU Freiberg, TU Braunschweig, …

2019 - 2021

Prof. Henning Wessels @TU Braunschweig

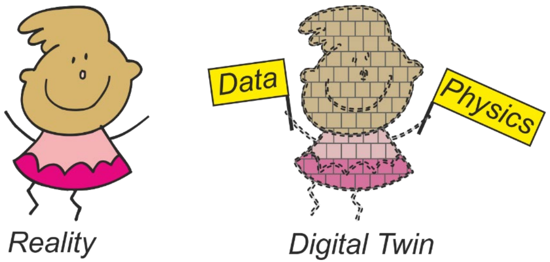
Data-driven modeling and simulation of mechanical systems

since May 2021

Proposal related to roadmap with Joachim Stahlmann and Ulrich Römer

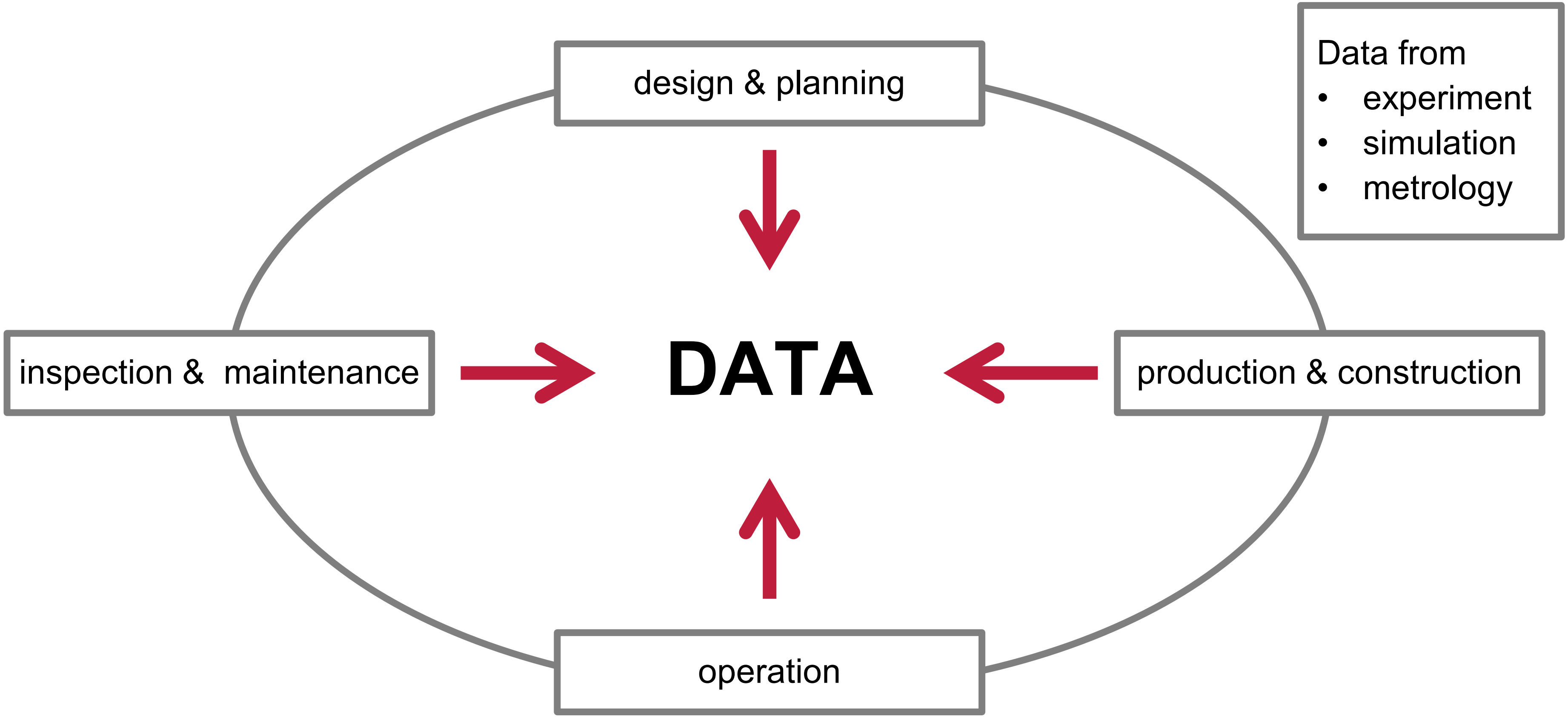
Dec 2021

Outline



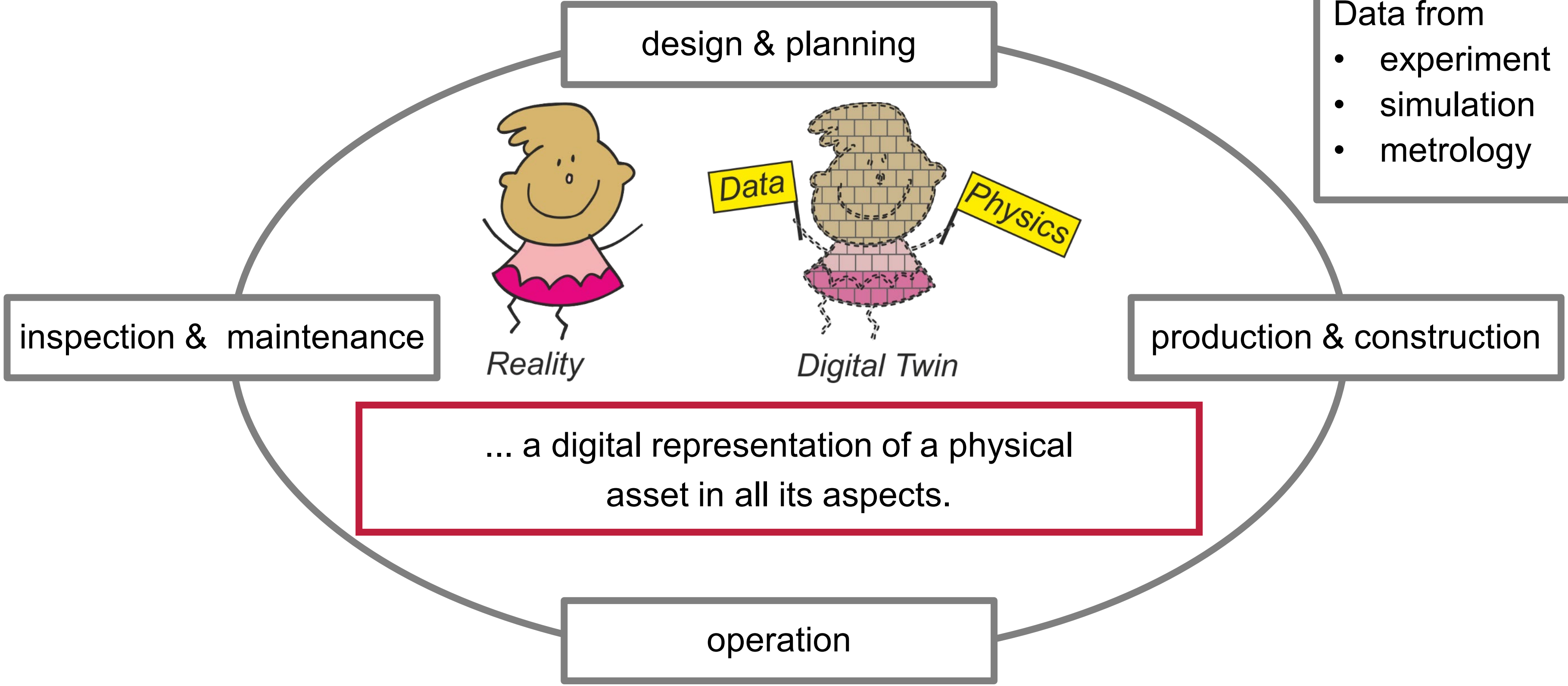
1. **Digital twinning of radioactive waste repositories**
2. Surrogate Modeling
3. Statistical Finite Element Method

1. A digital twin is …



1. A digital twin is …

Data from
- experiment
- simulation
- metrology



1. Digital twinning of radioactive waste repositories

IGG
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Joachim Stahlmann

iRMB

Jun.-Prof. Dr.-Ing.
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Institut für Dynamik und Schwingungen

Jun.-Prof. Dr.-Ing.
Ulrich Römer

- Geomechanics & Geotechnics
- Radioactive waste disposal
- Material modeling
- Monitoring

Physics-based model

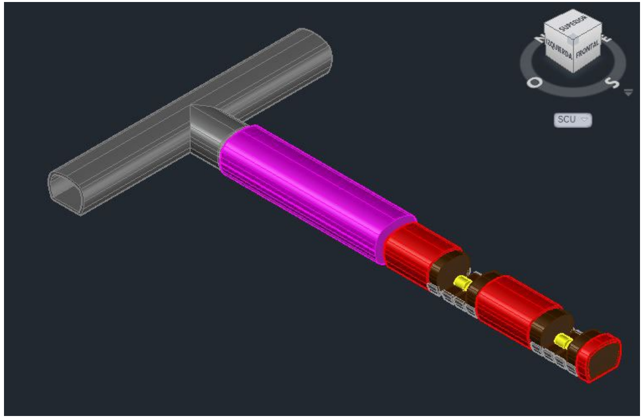
- Data-driven modeling and simulation
- Surrogate modeling
- Uncertainty Quantification

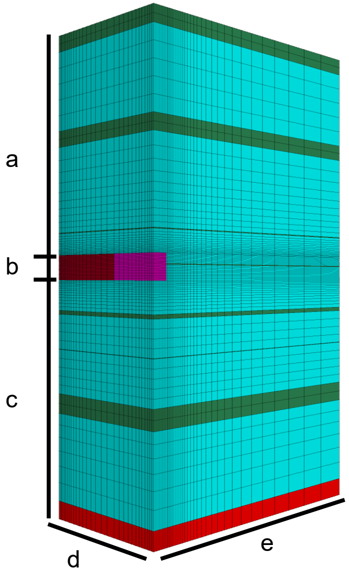
Data linkage

1. Geomechanical Modelling

Topology

Parametric virtual demonstrator





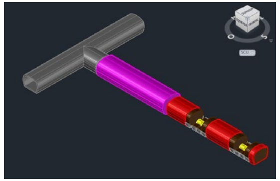
Variable parameter

- **Calibration** of material parameter
- **Optimization** of the repository's topology

1. Design loop

Calibration of material model parameters based on laboratory experiments

Optimization of storage drift with backfill and sealing plug



As-Planned

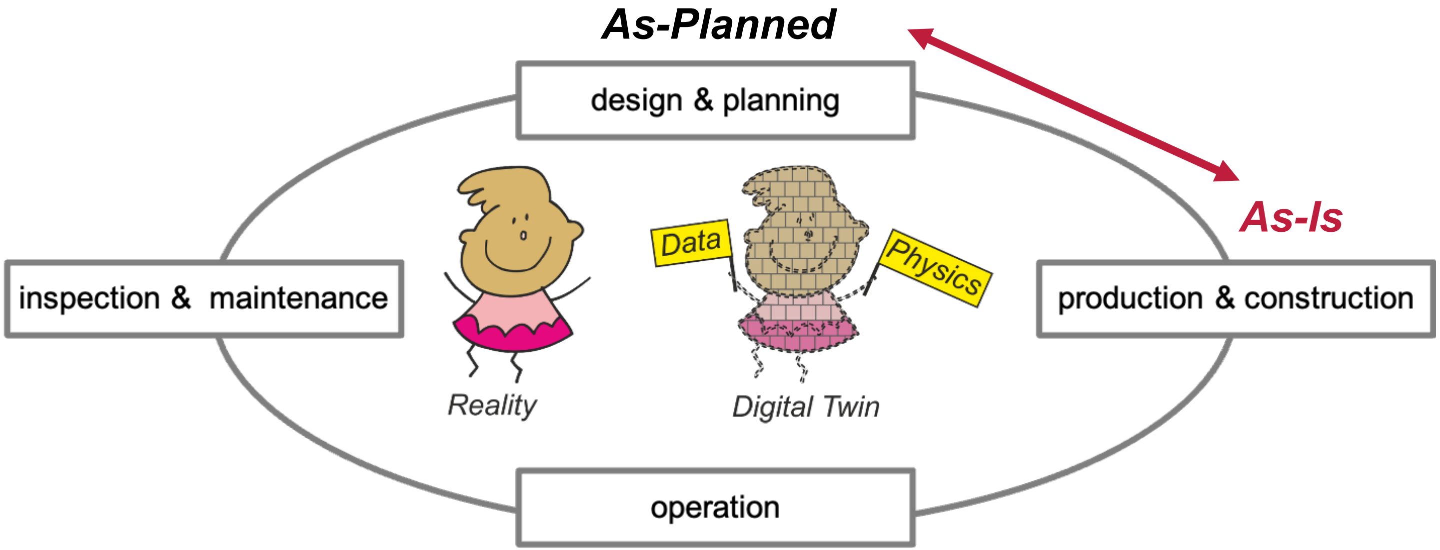
deteoriates from

As-Is

Planning I

Excavation

1. Design loop

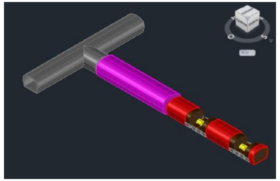


Planning I → Excavation → Planning II

1. Design loop

Calibration of material model parameters based on **lab experiments**

Optimization of storage drift with backfill and sealing plug



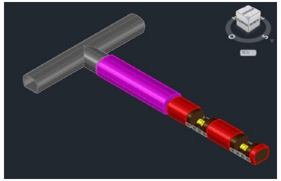
As-Planned

deteoriates from

As-Is

Calibration of material model parameters based on **monitoring data**

Optimization of storage drift with backfill and sealing plug



Planning I

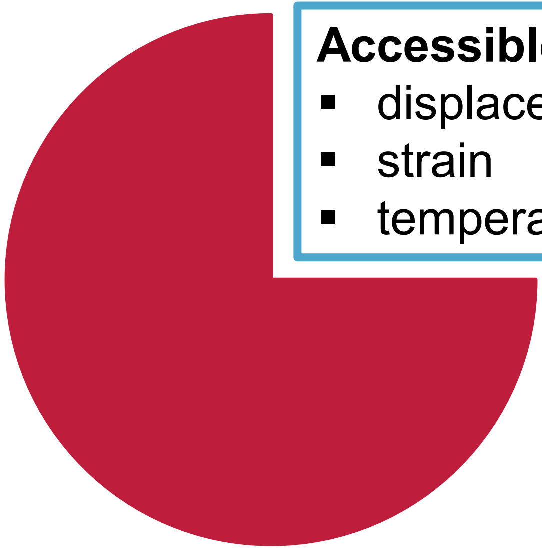
Excavation

Planning II

1. Why so complicated?

Sensors can only display a fraction of an entire system!

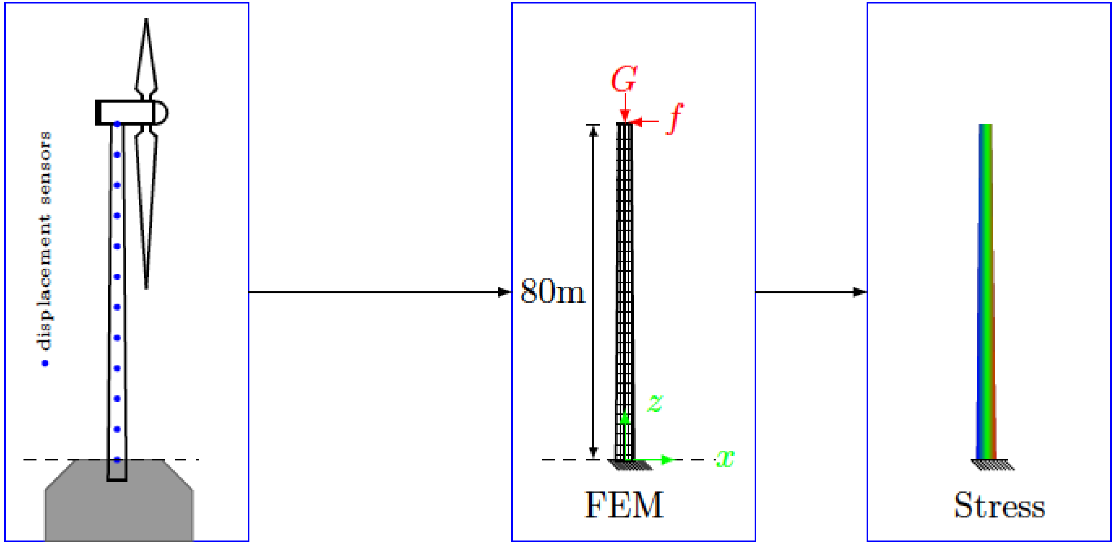
Inaccessible
- stress
- heat flux
- 3D fields of displacement/ strain/ temperature /…



Accessible via sensing
- displacements
- strain
- temperature

1. Why so complicated?

A well-calibrated model can provide otherwise inaccessible information.



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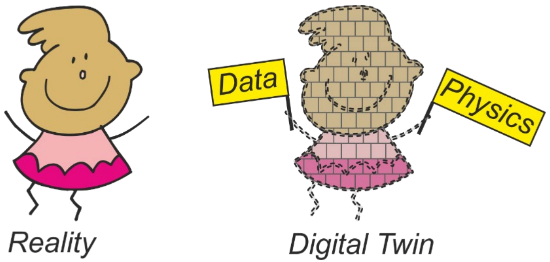
Inference of hidden quantities improves prognosis (extrapolation)!

Outline



1. Digital twinning of radioactive waste repositories
2. **Surrogate Modeling**
3. Statistical Finite Element Method

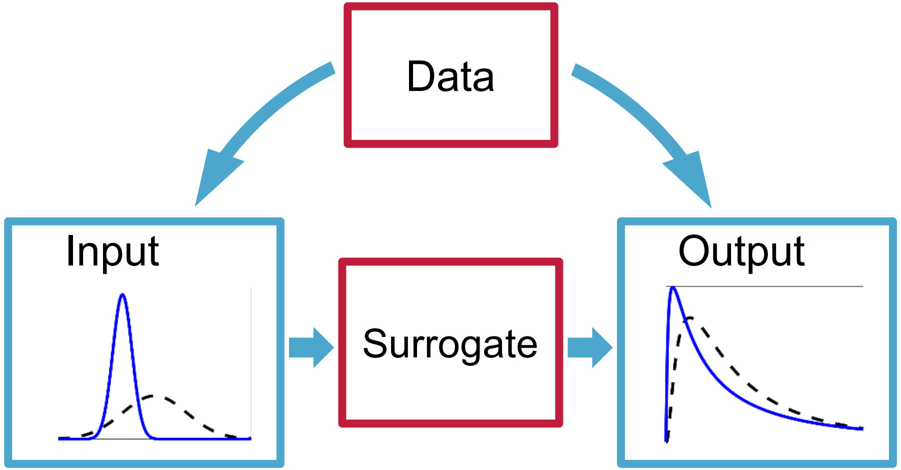
2. Surrogate Modeling

Input (Model parameter) → **surrogate model** (Virtual demonstrator) → **Output** (Quantity of Interest)

- Computation of the output Quantities of Interest (QoI) require expensive numerical simulations
- A metamodell can learn the functional relationship "*output = surrogate(input)*"
- Machine learning of the surrogate based on (input, output) data-pairs requires a once only a high computational invest (training)
- Gaussian processes enable efficient training (adaptive sampling of design points)

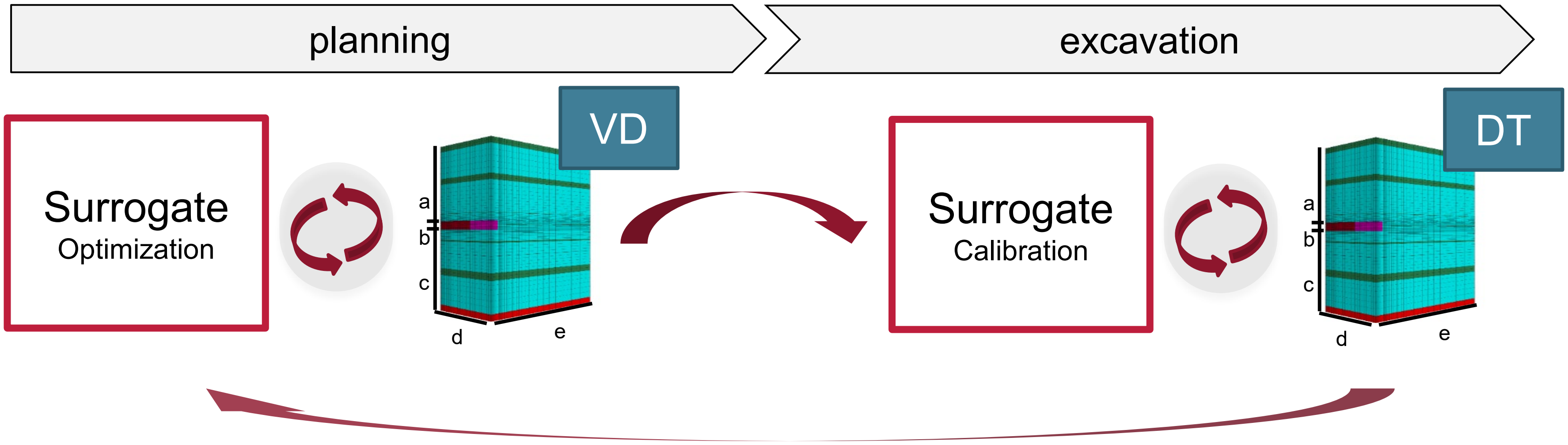
2. Calibration

- Reality is represented by monitoring data, e.g. storage drift
- Discrepancy between measured δ_i^{mess} und simulated drift $\delta_i^{sim}(\mathbf{p})$ is expressed by an objective function
$$L = \sum_{i=1}^{n} |\delta_i^{mess} - \delta_i^{sim}(\mathbf{p})|^2$$
- Calibration → minimization of the objective function to fit the model parameter to measurement data



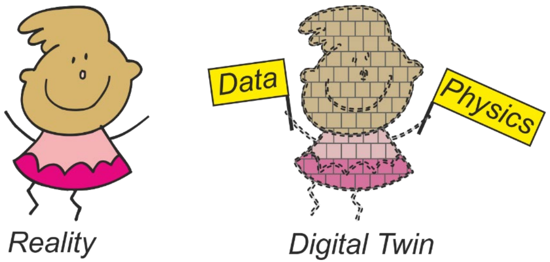
Surrogate modelling reduces computational cost within the calibration loop

2. Digital Twin



Goal: The **Virtual Demonstrator (VD)** and the monitoring data reflect as **Digital Twin (DT)** the reality and support constructive decisions

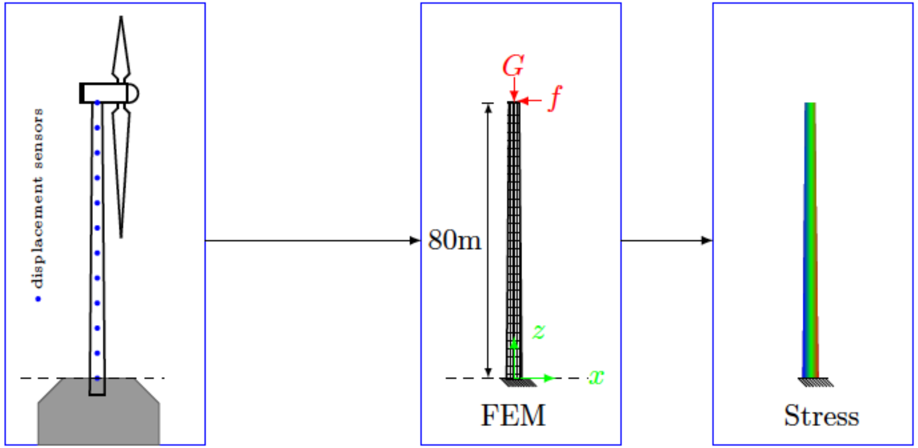
Outline



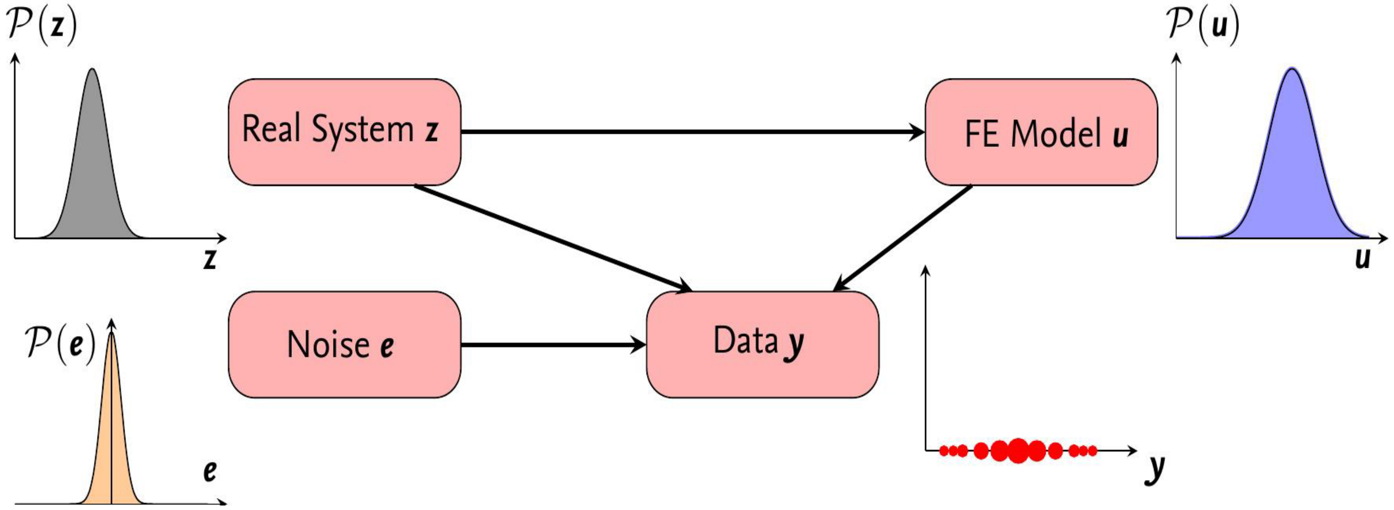
1. Digital twinning of radioactive waste repositories
2. Surrogate Modeling
3. **Statistical Finite Element Method**

3. Motivation

- Engineering systems are designed using deterministic mathematical models that are often discretized and solved with FEM
- The uncertainties in geometry, loading and material are taken into account through safety factors or stochastic approaches
- However, there is no statistically coherent way of getting data into FEM simulations

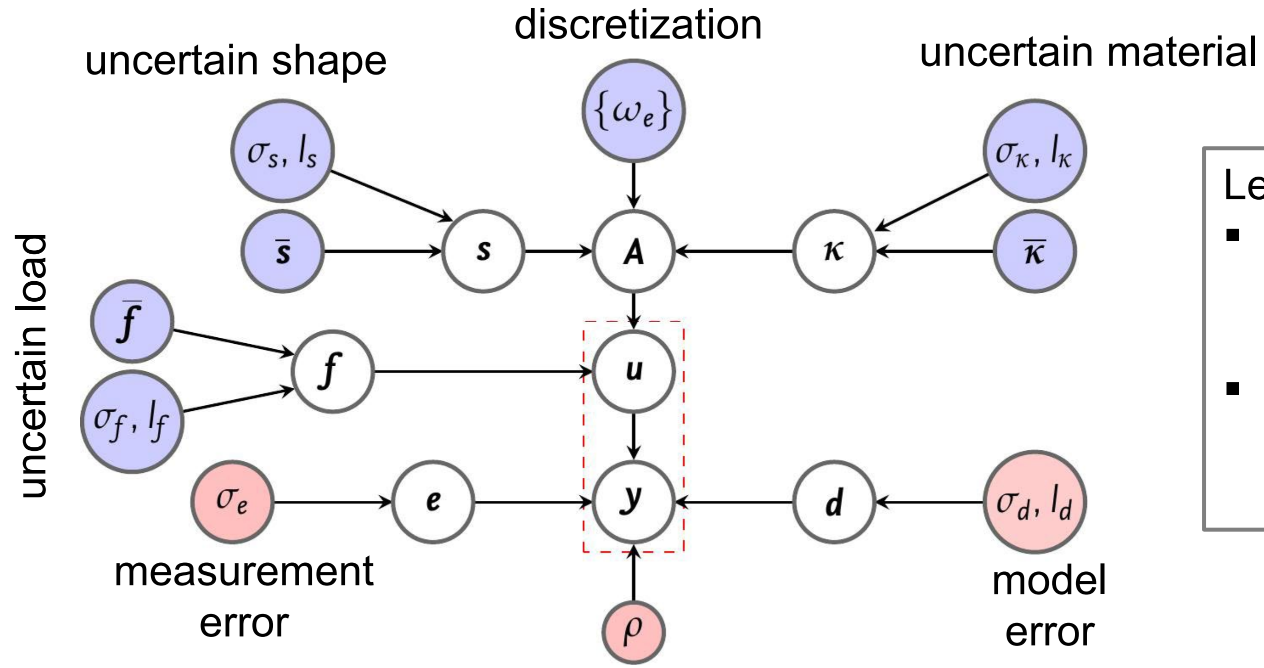


3. Statistical Finite Element Method



The quest for truth (aka the real system)

3. Statistical Finite Element Method



Legend
- Blue circles: model uncertainties → non-trainable parameters
- Red circles: statistical generating parameter → trainable

[Girolami, Febrianto, Cirak (2021)]

3. Bayes’ Theorem

$$p(\mathbf{u}|\mathbf{y}_{\mathrm{obs}}) \propto p(\mathbf{y}_{\mathrm{obs}}|\mathbf{u})\ \mathbf{p}(\mathbf{u})$$

$p(\mathbf{u}|\mathbf{y}_{\mathrm{obs}})$: posterior distribution

Given the data $\mathbf{y}_{\mathrm{obs}}$, what is the probability of $\boldsymbol{\theta}$

$p(\mathbf{y}_{\mathrm{obs}}|\mathbf{u})$: likelihood

Under the assumption of $\mathbf{u}$, what is the probability of observing the data $\mathbf{y}_{\mathrm{obs}}$

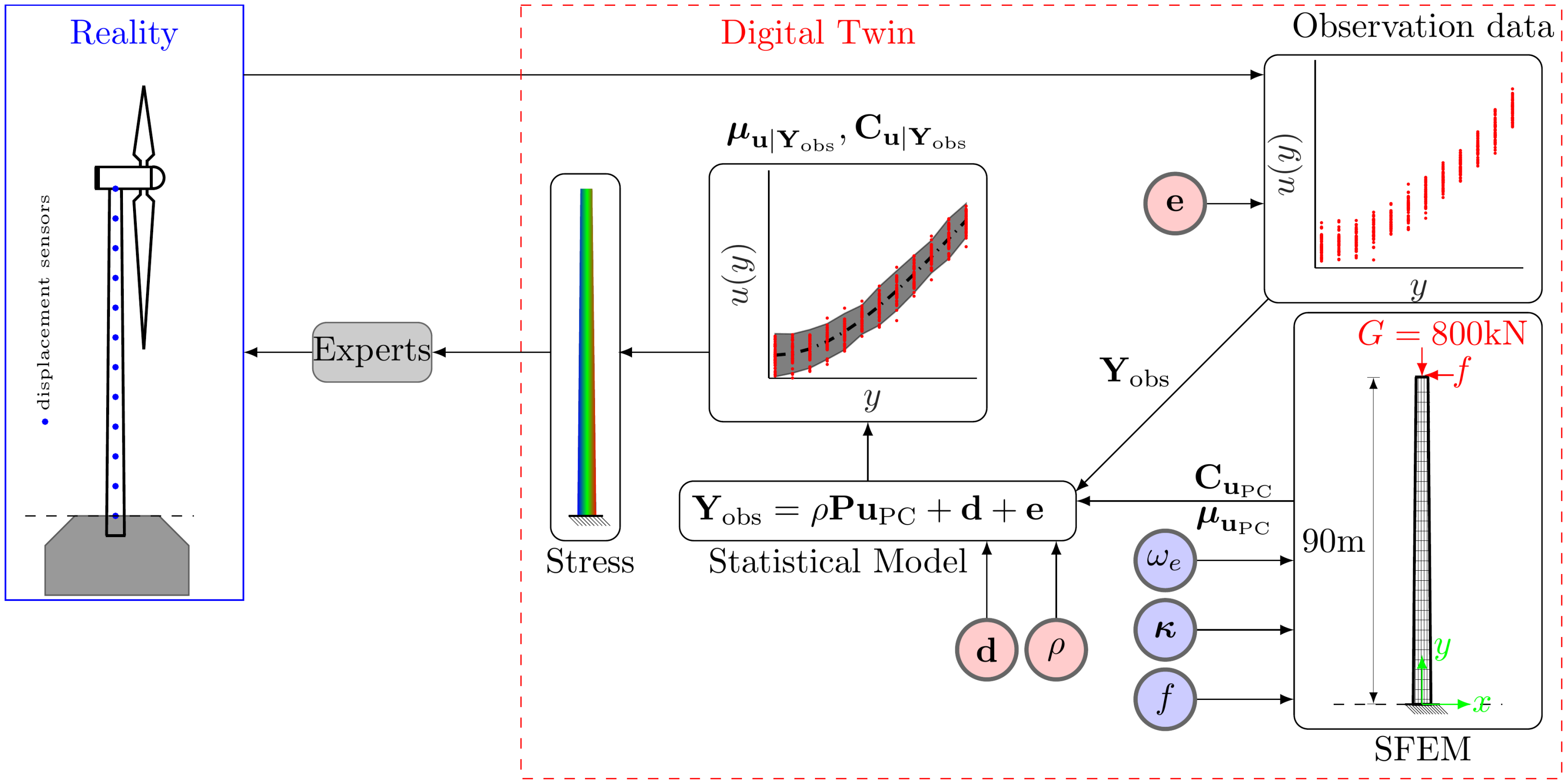
$p(\mathbf{u})$: prior distribution

Knowledge about $\mathbf{u}$ before updating

$\mathbf{u}$: simulated stochastic displacement

$\boldsymbol{\theta}$: observed noisy displacement

3. Statistical Finite Element Method



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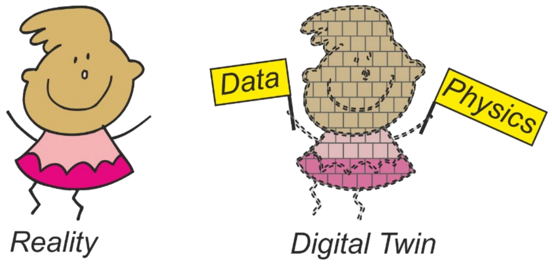

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Summary

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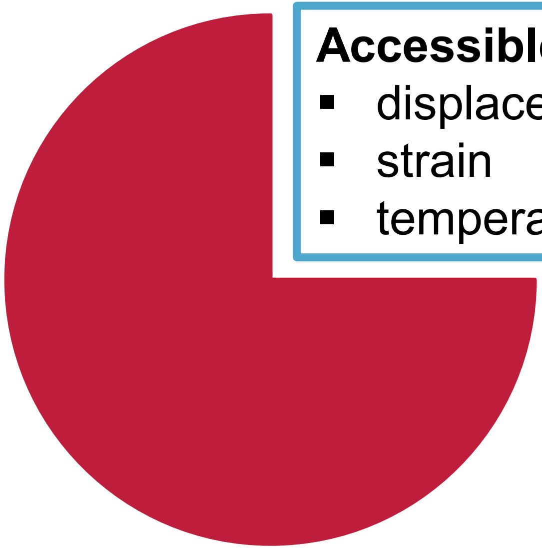

Accessible via sensing
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Summary

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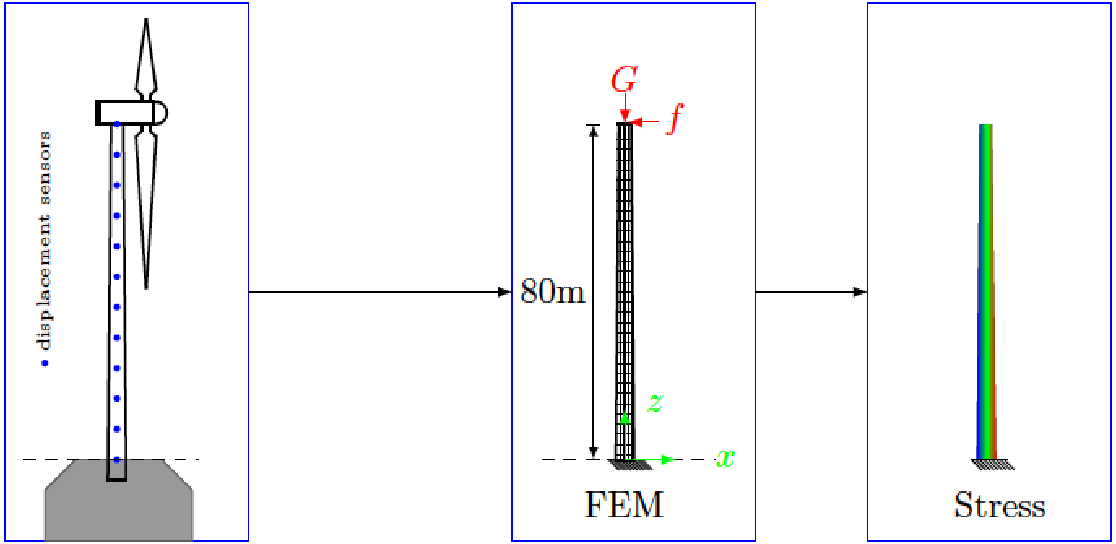

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