PREDIS

PAUL SCHERRER INSTITUT PSI

NRG

Digital Twins in PREDIS

A digital Twin/Tool for waste package evolution

G. DAN MIRON[2] (DAN.MIRON@PSI.CH)

HANS MEEUSSEN[1], WILFRIED PFINGSTEN[2], JAN TITS[2], SERGEY V. CHURAKOV[2]

Partners in PREDIS: BAM, [1]NRG, KIT-INE, Amphos-21, Magics, SCK-CEN, [2]PSI

EURAD-PREDIS Digital Twins Webinar 16th of February 2022

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 945098.

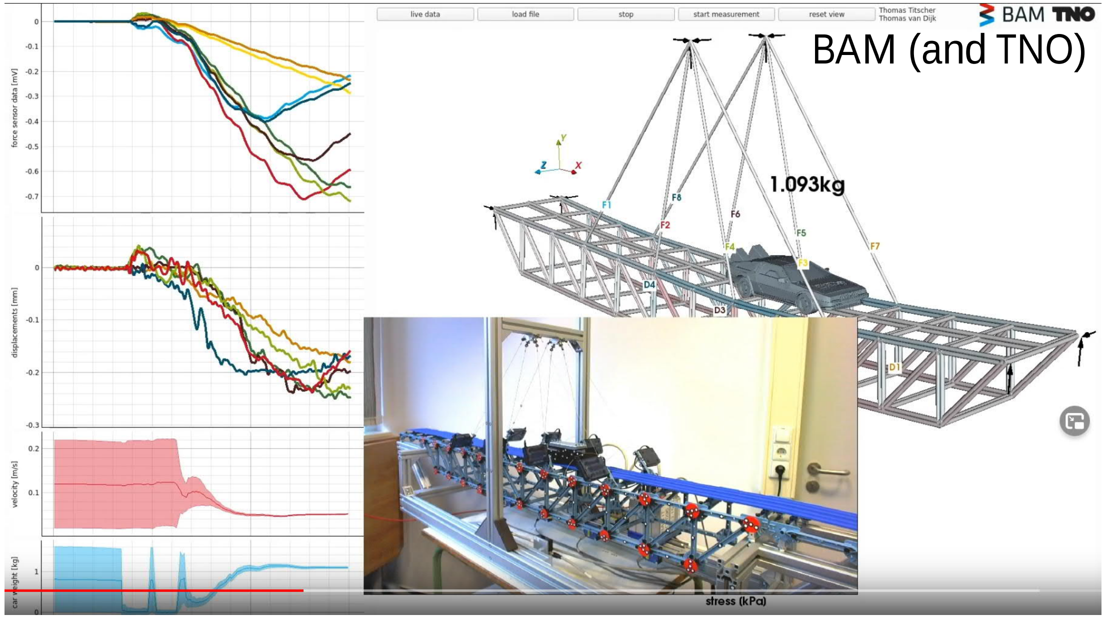
Digital Twin

- What is a digital twin and challenges?
- What is the purpose of the PREDIS digital twin?
- What are input and output parameters?
- How can detailed geochemical process models be integrated in it?
- Technical implementation

This project has received funding from the European Union's Horizon 2020
research and innovation programme under grant agreement No 945098.

Digital Twin – virtual replica – real time update

Mandi (2019): “A Digital Twin is a virtual instance of a physical system (twin) that is continually updated with the latter’s performance, maintenance, and health status data throughout the physical system’s life cycle.”



https://www.youtube.com/watch?v=ReWmrbQgQLU

- **Digital image** of the system
- **Layers of information** (sensors, real time update)
- **Simulation models** to predict the future behavior based on previous data

Example

- Digital twin aimed at improving the **monitoring and maintenance of bridges**
- Changes happen on the **scale of seconds**, minutes, hours

This project has received funding from the European Union’s Horizon 2020 research and innovation programme under grant agreement No 945098.

Digital Twin – long term evolution - challenges

Adapted from Bankhead et al. (2018): A digital Twin is a **framework capable of predicting** the most important variables of a physical asset, built from **several components** (models) **integrated into a single powerful tool** that enables the end user to **predict the outcome of scenarios**, predict the values of outputs as a function of the inputs.

- Changes that happen in waste packages are related to **chemical processes that happen very slowly**:
  - ion diffusion, degradation of organic matter, corrosion of metals, mineral dissolution/precipitation

We want to model **the evolution on scales of tens of years of very slow processes**

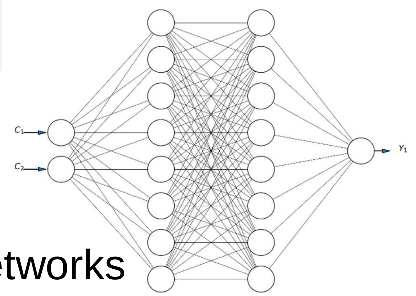
Combine **data from different sources (experiments, monitoring, modeling), use data from/in different codes and models** developed by different partners – data managing, documenting workflows and dissemination to end-users

A **proof of concept having digital twin functionalities** with the possibility to build upon.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 945098.

Digital Twin – Digital tool

- A **friendly and accessible tool specifically designed** for assessing / predicting different **waste package evolution scenarios**
- A selection of **independent and/or coupled processes** related to the mineralogical and mechanical properties evolution (usually a few are responsible for main changes).
- Full thermal-hydrological-mechanical-chemical (THMC) coupling is not foreseen.
- Running different geochemical and chemo-mechanical models for given waste package properties (input) to retrieve **parameters (output) relevant for waste package integrity evolution as a function of time**
- **Use of surrogate models** (e.g., trained neural networks, lookup tables, simplified empirical functions) for accounting for different degradation processes – exchange with **EURAD DONUT**



deep neural networks

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 945098.

A PREDIS Digital Twin

- Ability to **run processes on different compositions**, generate a **dataset of waste package evolution** scenarios.
- Set of **reference waste types and predefined compositions** setup and modeled by experts accessible to the end-users.
- **Fill gaps due to limited information** available from existing waste packages with provided predefined compositions.

Use for:

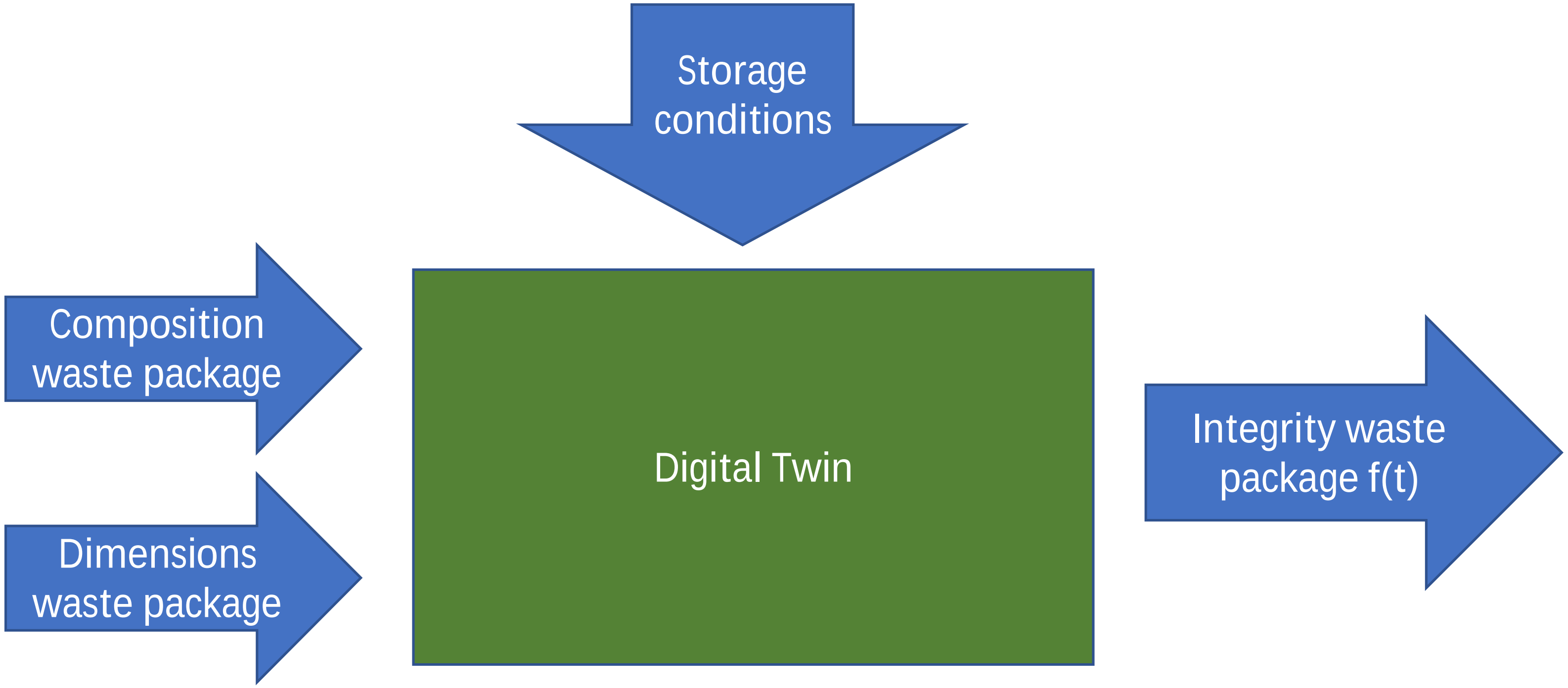
- **Legacy waste packages** to evaluate many different “what if scenarios”.
- **Upcoming/future waste packages** to test different compositions for potential problems (e.g., suitable aggregates, new phosphate rich cements)

Statistical Models:

- **Monte-Carlo based uncertainty propagation** – probability that output properties exceed a threshold based on sampling the input parameter distribution.
- **Global Sensitivity Analysis** – rank input parameters based on their influence on the model output

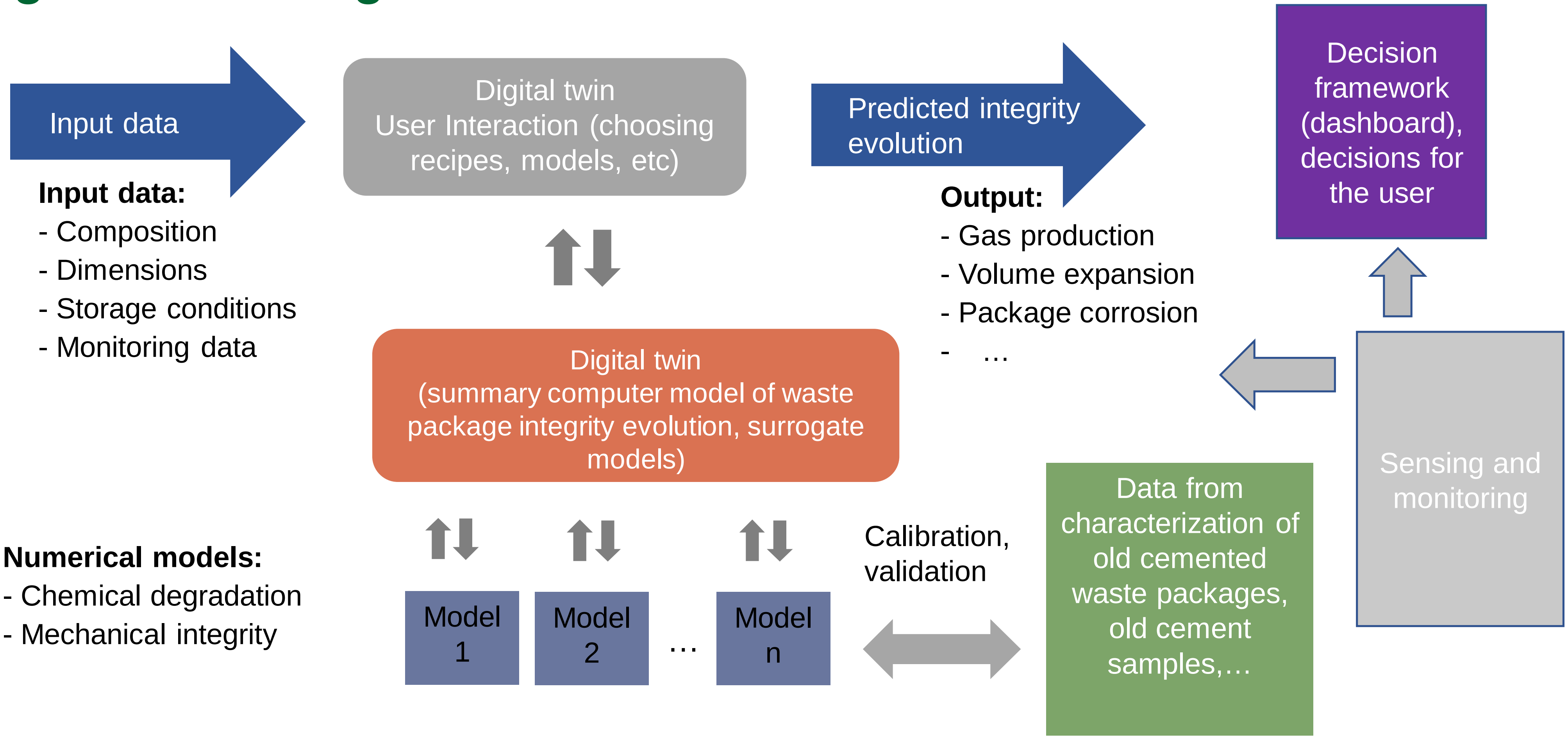
This project has received funding from the European Union’s Horizon 2020 research and innovation programme under grant agreement No 945098.

Overview functionality Digital Twin

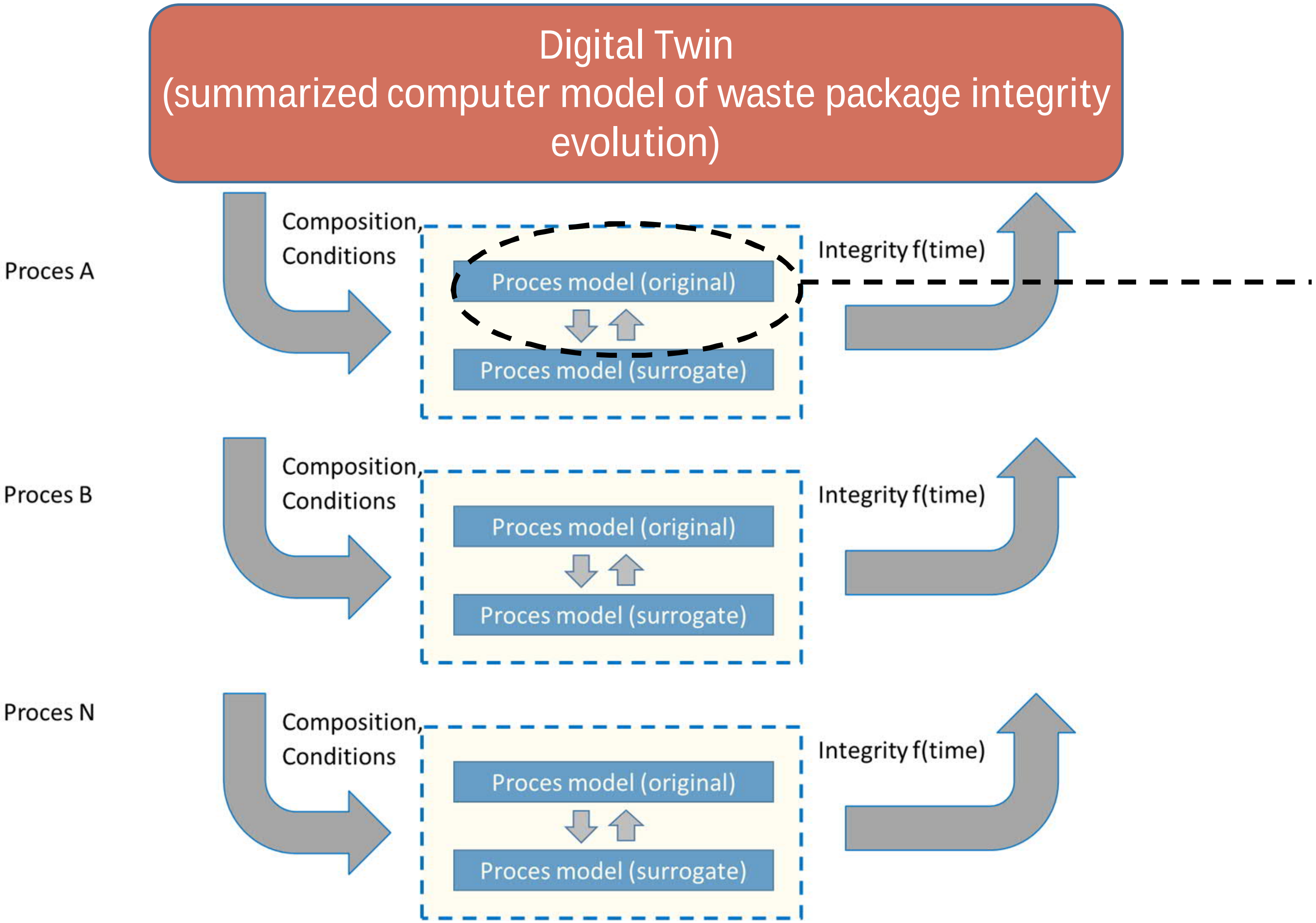


This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 945098.

Digital Twin – Digital tool



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 945098.



Example implementation

- Cement carbonation model
- 2D cementitious material

Input:

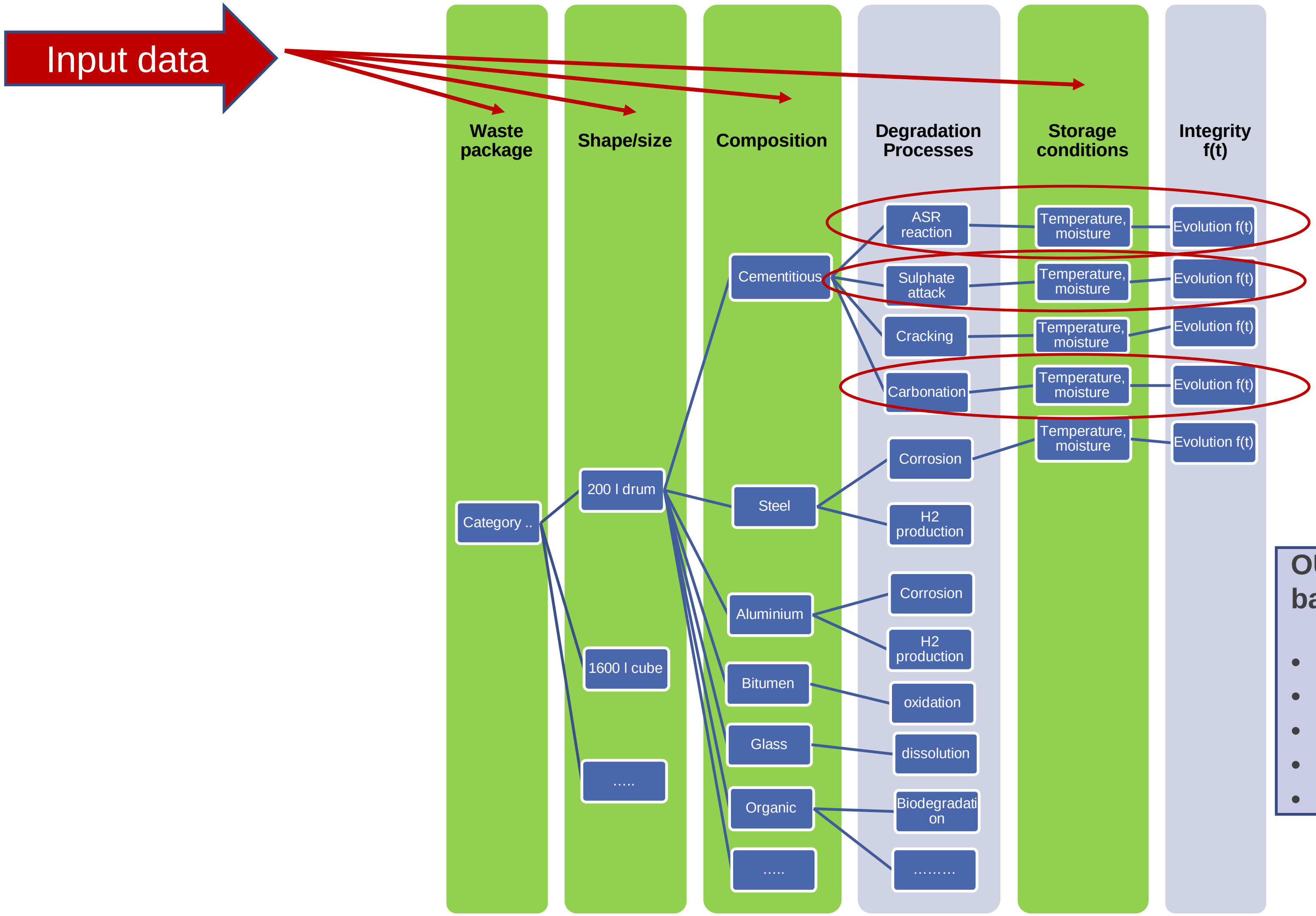
- Cement composition
- Chemical/physical
- CO_2 pressure boundary condition

Output:

- Measure of integrity f(t)

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 945098.

Surrogate models as process simulatiors



surrogate ASR model
(e.g.trained on SCK model)

surrogate sulphate attack model
(e.g. trained on NRG model)

surrogate carbonation model
(e.g. trained on A21 model)

OUTPUT data Integrity f(t), based on e.g.:

- Pressure build up
- Surface expansion
- Stress
- Cracks
- Porosity changes

Digital Twin – Technical Implementation

- **Input/output ascii/text files in CSV format** (easily convertible to other formats to be uploaded in a database), data from files or a database (public or private), metadata, workflows automation/documentation
- **Use of preferred modeling tools** (geochemical, reactive transport, mechanical) that can communicate through programing interfaces (C++, python) or files (meta data on modeling problem setup), and are triggered by the digital twin to do calculations
- **Use of Jupyter notebook development environment** (web-based, collaborative interactive development environment, works in the browser) – through python access to numerous libraries (statistics, graphical interface, visualization)
- **Open-source code development**, collaboration between partners **using git (all contributions visible)**
- Can be run on an online platform (e.g. **GeoML.eu**, google colab, binder, setup on Azure) or installed and run on a local machine (use of sensitive data)

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 945098.

GeoML.eu JupyterLab service

Digital Twin – Development platform

For users:
For developers:

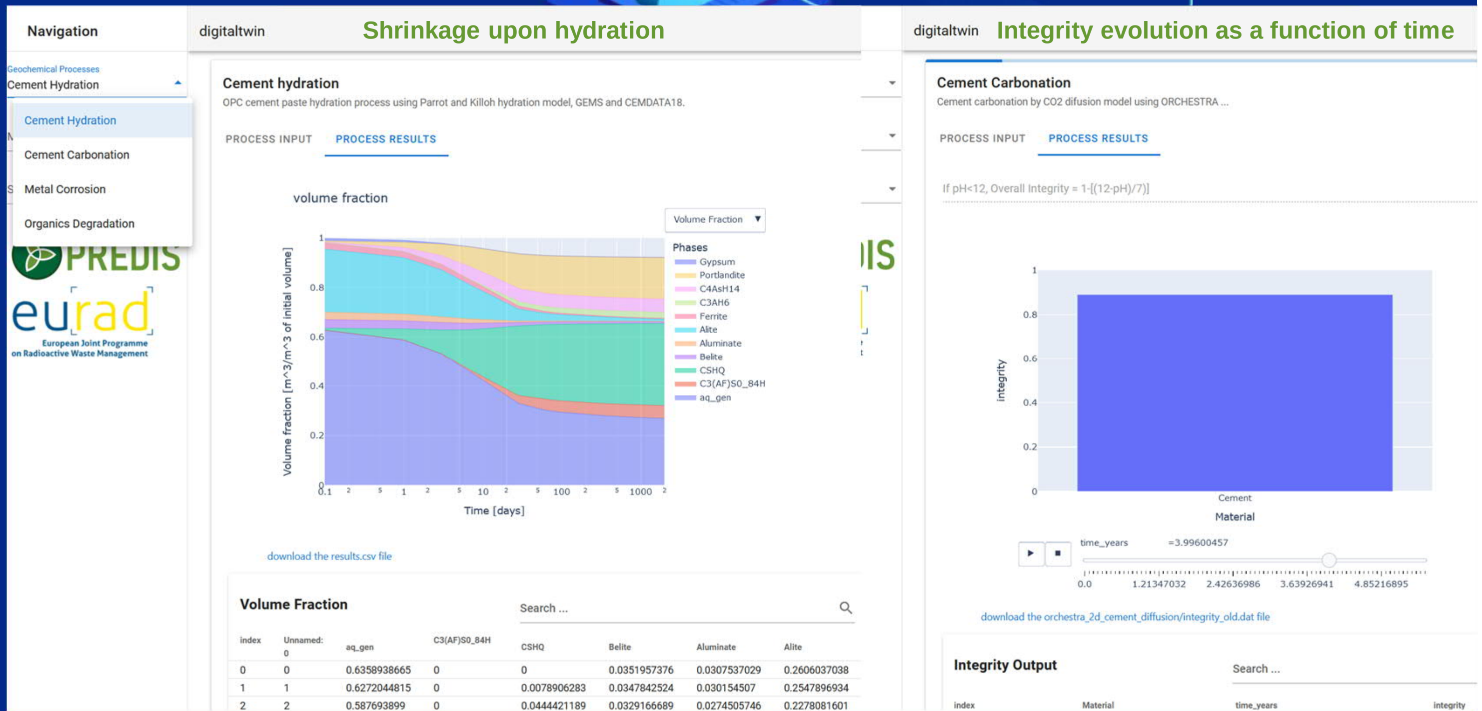
- No computing resources? No problem!
- No need to install any software on your device
- JupyterHub will work via your web browser
- Go into one of lab folders and open a notebook
- Create your own lab folder and Python environment
- Launch your advanced demo app on a Voila server
- Various ways of collaboration are possible

For participants of EURAD projects!

LOGIN TO OUR JUPYTERLAB

Predis Demo: Digital Twin

START DIGITAL TWIN DEMO



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 945098.