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hereon

Open Model develops and provides to European Industry a comprehensive, integrated **open modelling framework** for accelerated innovation processes and development of **novel materials and products**. Validation in Open Model includes standardized workflows to quickly and reliably test materials models and solvers, benchmarks efficient comparison with measurements, and close integration with experimental design.

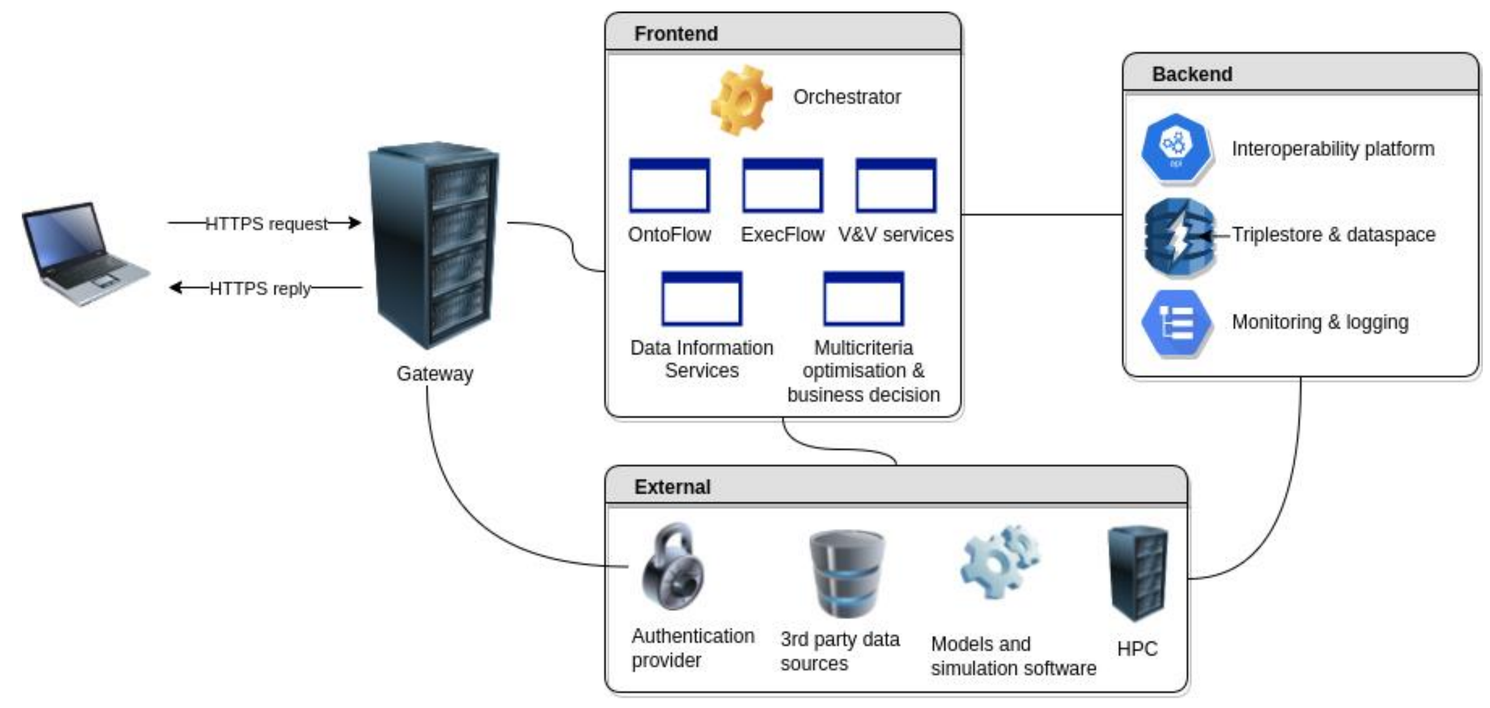

Fig. 1: Open Model Platform Overview

Goals

- Develop OIP based on established technologies like Dlite and AiiDA
- Allow the easy integration of optimization and validation in existing workflows
- Develop methodology to select models based on KPIs
- Create framework to efficiently implement ontology based workflows
- Cooperate with EMMO to further develop ontologies for workflows and models

Use cases at hereon

Optimization of protective interface layer formation in novel aluminum reinforced concrete

In cooperation with: Hydro SINTEF

Using aluminum reinforcements in cement allows for further design possibilities and lightweight design of structures. The high PH value of conventional cement prevents the direct use of aluminum reinforcements. As such a novel clay-based cement [1] is used in this case.
Furthermore, aluminum allows the use of extrusion making it possible to use different reinforcement shapes (see Fig. 3) to **optimize the mechanical performance**.
To increase the longevity of structures a model is developed to predict the **corrosion protection performance** of the cement-aluminum layer.

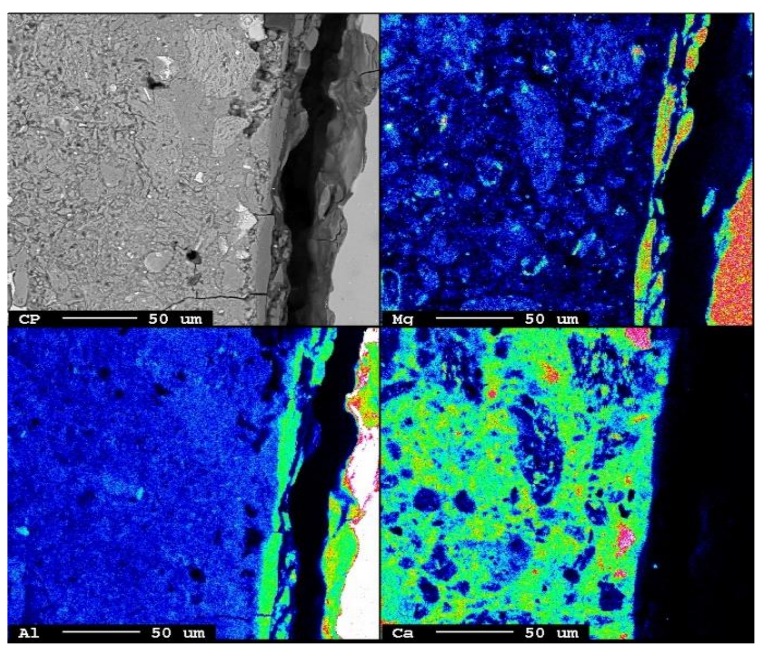

Fig. 2: Microscopic images of the aluminum-cement interface layer. [1]
Left top: Black-white,
Right top: Mg concentration,
Left bottom: Al concentration,
Right bottom: Ca concentration

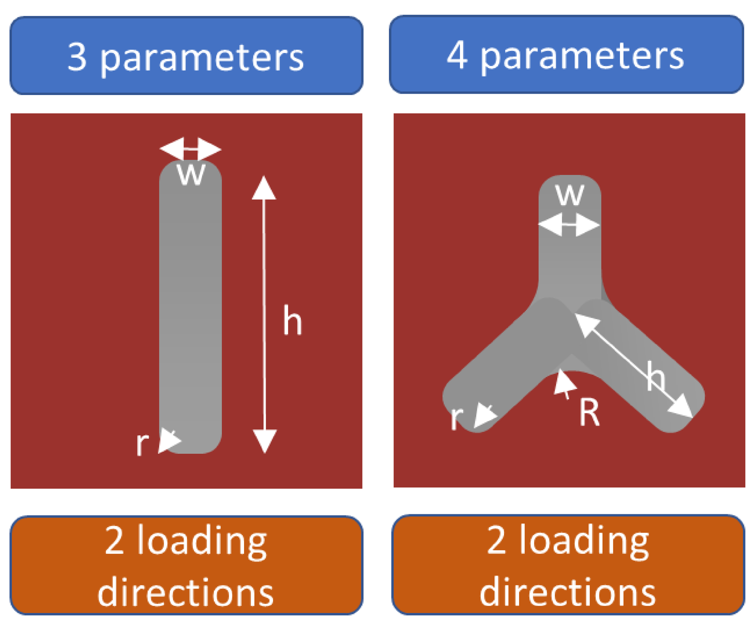

Fig. 3: Examples of proposed extruded aluminum reinforcement shapes.

[1] H. Justnes and T. Danner: Microstructure of Cement/Clay paste with Aluminum bar after 1 year storage in Fresh Water and in 6% NaCl, 2021
[2] www.aspherix-dem.com

Data-based optimization of metal processing

This use case aims to optimize the processing parameters of metal materials, for example, in extrusion or rolling, and predict the resulting material's physical properties.
A database of different processed alloys and testing results has been assembled to generate an ML model to predict the resulting physical properties for untested alloys and extend the model quality to larger process parameter ranges.
Preliminary results are shown in Fig. 4 and 5.

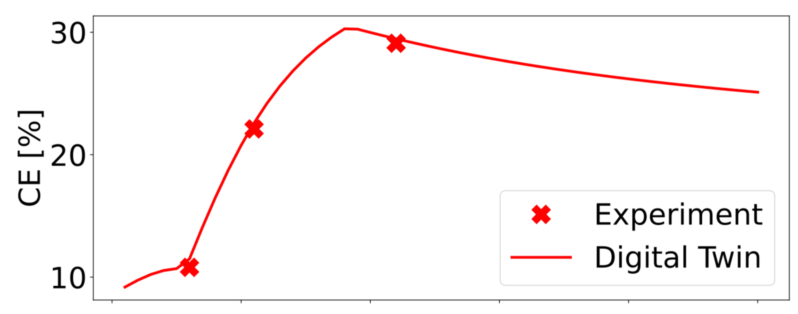

Fig. 4: Validation of the ML model.

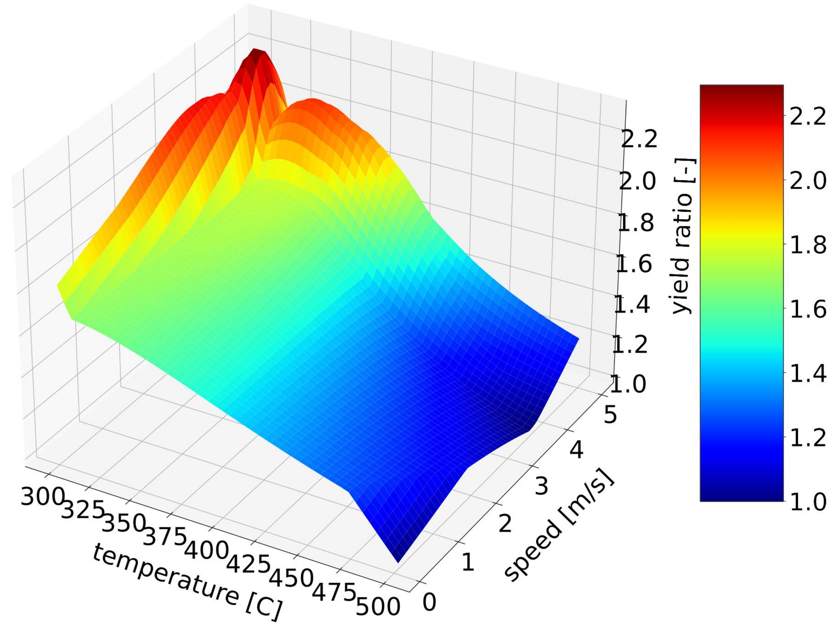

Fig. 5: Process-parameter-material-propery map for the yield ratio [TYS/CYS] for a Mg-Gd alloy generated using the ML model.

Optimization of the micro porous layer in fuel cells

In cooperation with: DCS COMPUTING TOYOTA

The aim of this use case is the optimization of the micro porous layer (MPL), which has a large impact on the performance of the gas diffusion layer (GDL) of a fuel cell. As such effectively modeling and optimizing the performance of a fuel cell depends greatly on the quality of the MPL.
Aspherix DEM [2] is used to generate the MPL geometry and to model the performance of the GDL in regards to such parameters as fiber size and orientation.
Fig. 6 and Fig. 7 shows some of the preliminary results of the model.

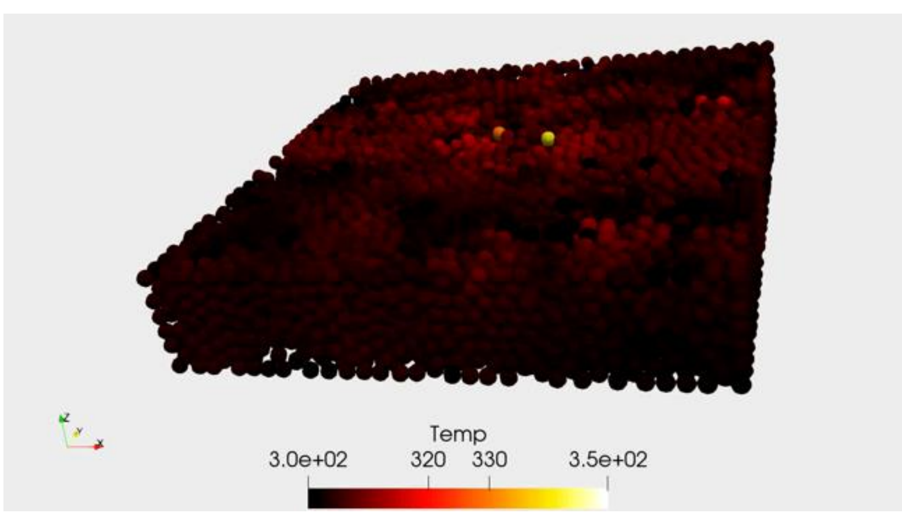

Fig. 6: Temperature distribution in the MPL.

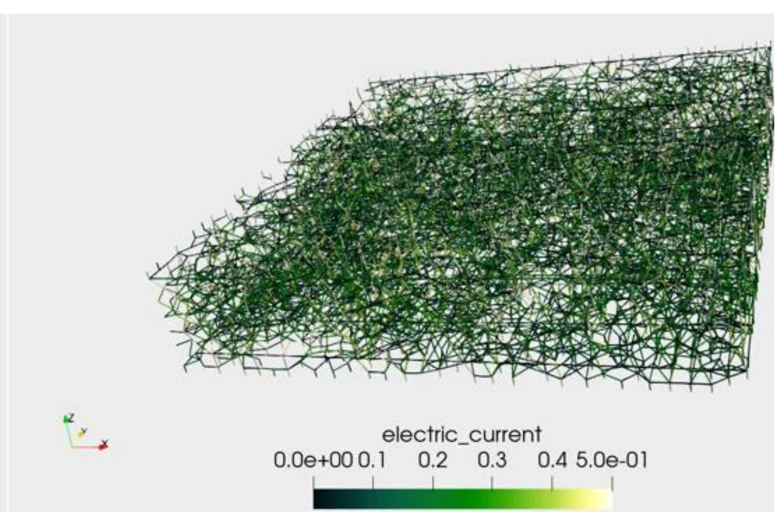

Fig. 7: Electrical current distribution in MPL.

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