TECHNISCHE UNIVERSITÄT DRESDEN
NTNU Norwegian University of Science and Technology
SINTEF
LUXEMBOURG INSTITUTE OF SCIENCE AND TECHNOLOGY LIST

MEDIATE

A Semantic-based Material Twin and Co-Simulation Platform for Solid Oxide Fuel Cells

MEDIATE

Eric Langner[1], Mohamed El Hachemi[2], Hamidreza Dehghani[2], Artem Semenov[1], Thomas Wallmersperger[1], Sylvain Gouttebroze[3], Casper W. Andersen[4], Heinz A. Preisig[5] and Salim Belouettar[2]

[1] TU Dresden, Institute of Solid Mechanics, Dresden, Germany
[2] Luxembourg Institute of Science & Technology, Luxembourg
[3] SINTEF, Trondheim, Norway
[4] SINTEF Ocean, Trondheim, Norway
[5] NTNU, Department of Chemical Engineering, Trondheim, Norway

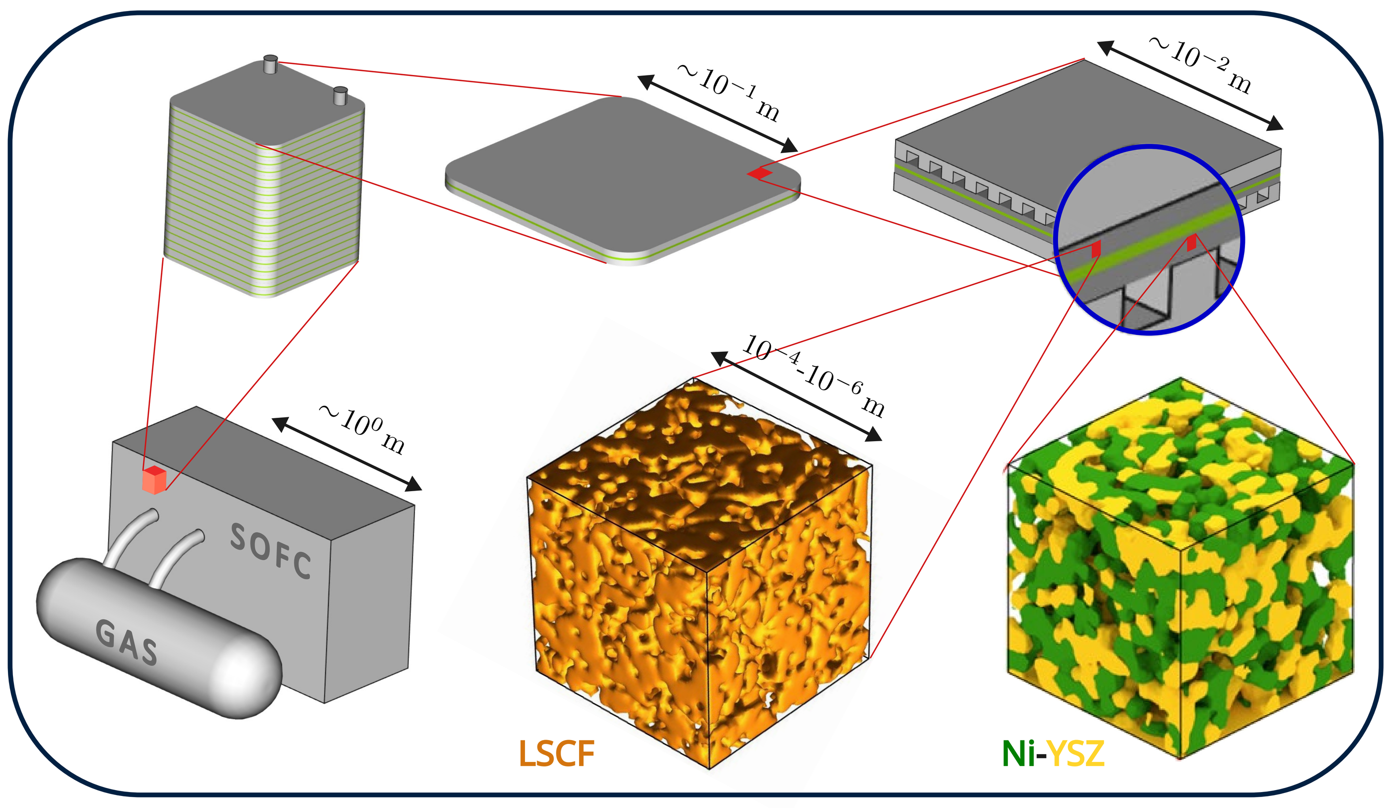
Project description

The **MEDIATE** project develops an advanced knowledge-assisted platform to optimize solid oxide fuel cell (SOFC) performance by combining physics-based modeling with machine learning (ML). This approach enhances predictive accuracy, efficiency, and durability while reducing computational costs.

A framework was developed to **investigate** the **porous microstructures** of SOFC electrodes. The geometrical properties (including tortuosity, percolation, statistical correlation functions) are analyzed that leads to certain effective physical quantities, such as conductivities, permeability and mechanical behavior including creep. Additionally, a methodology was developed to generate or reconstruct 3D microstructures of SOFC anodes and cathodes that can be used to enrich the database for inverse design approaches.

A **macroscopic, multiphysical SOFC model** captures mass transport, electro-chemical reactions, thermal and mechanical behavior including creep. The model contains the effective properties from the microstructural investigations. High-fidelity simulations generate synthetic datasets to train **artificial neural networks** (ANNs), predicting key SOFC performance metrics, including temperature distribution, gas concentration, and current density. Time-dependent simulations further analyze SOFC behavior under dynamic conditions.

The **platform**, anchored in the Elementary Multi-perspective Material Ontology (EMMO), ensures seamless data exchange and real-time performance optimization. By merging physics-based insights with ML techniques, this project contributes to the development of high-performance, sustainable fuel cell technologies.



SOFC analysis at different length scales

Microstructure analysis [1,2]

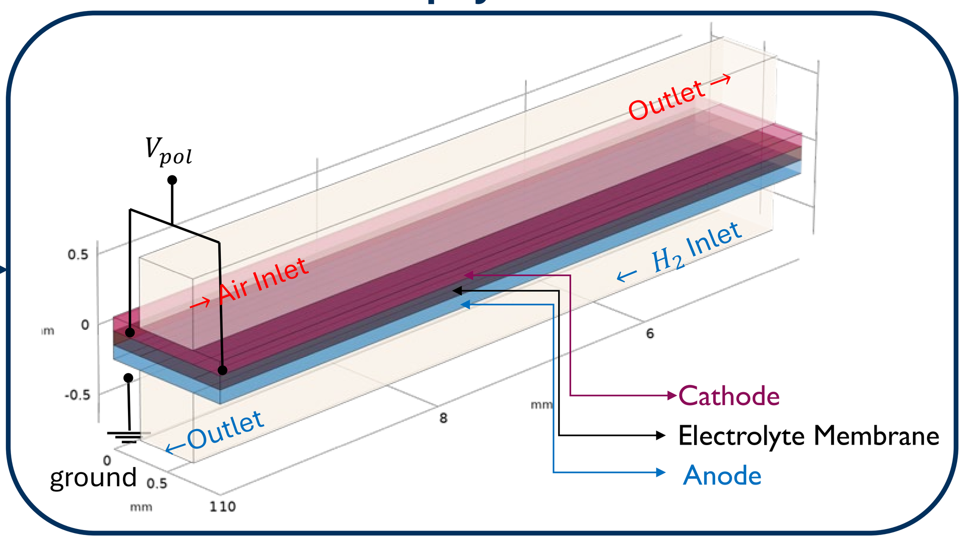
Geometrical parameters
- Volume fraction
- Tortuosity
- Triple Phase Boundary
- Percolation
- Two-point correlation function
- Lineal-path function

Computational homogenization

Physical quantities
- Conductivities
  - Thermal
  - Electric
  - Ionic
- Fluid permeability
- Inelastic mechanical behavior
  - Stiffness
  - Thermal expansion
  - Creep

Macroscopic modeling [3,4,5]

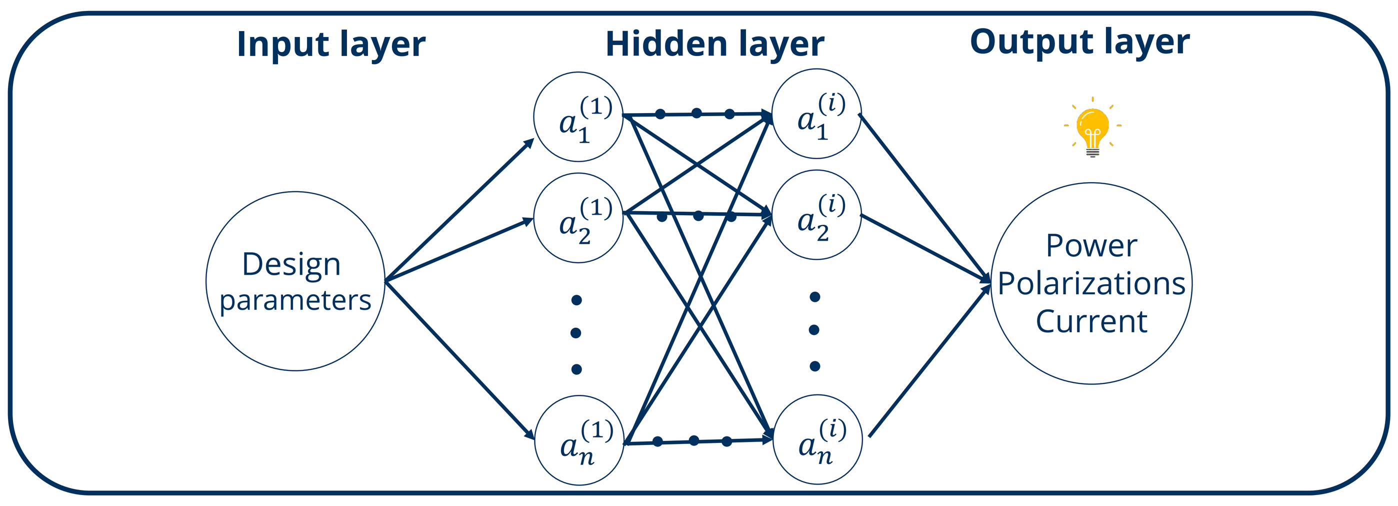
Multiphysical model



- Mass transfer
- Charge transfer
- Momentum transfer of fluid
- Species conservation
- Energy conservation
- Momentum balance of solid

Artificial neural networks [4]

Creating a large data base for an ANN with various design parameters
- Geometrical parameters of the single fuel cell
  - Gas flow channel dimensions
  - Membrane layer thicknesses
- Electrode properties
- Operating parameters
  - Operating temperatures
  - Pressure drop at electrodes



Semantic platform [4]

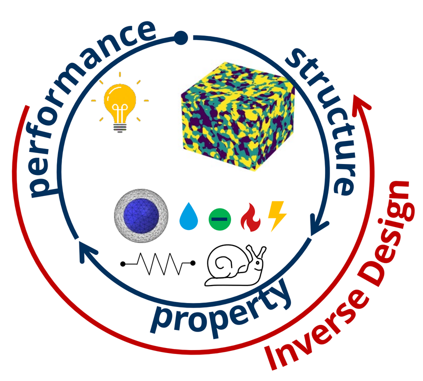
Simulation/Modeling (Physics-based) ↔ **Data Exchange** (EMMO) ↔ **Optimization/Control** (ML-driven)

Structured ontology framework
- Standard data representation
- Interoperatbility between models and tools
- Real-time data exchange and feedback
- Facilitates knowledge integration

Outlook

Current work
- Inverse design for optimal electrode microstructures
- Further implementation of structure-property-performance linkages into the platform

Future perspectives
- Include manufacturing process into the framework
- Optimization of SOFC to maximize performance and long-term durability



References:
1. Langner, E., Makradi, A., El Hachemi, M., Belouettar, S, Wallmersperger, T. "Determination of the effective conductivities of solid oxide fuel cell electrodes using the first-order homogenization method." PAMM 23.2 (2023): e202300105.
2. Langner, E., Semenov, A., Makradi, A., Gouttebroze, S., Belouettar, S., Wallmersperger, T. "Macroscopic properties of solid oxide fuel cell electrodes via microstructure-based numerical homogenization." PAMM 24.4 (2024): e202400023.
3. Makradi, A., El Hachemi, M., Langner, E., Belouettar-Mathis, E., Lengiewicz, J., Wallmersperger, T., Deghani, H., Preisig, H., Gouttebroze, S., Andersen, C. W., Småbråten, D., Belouettar, S. "3D and time-dependent simulation of a planar solid oxide fuel cell: Bridging Microstructure and Multiphysics Phenomena". Acta Mechanica. 2025 (submitted).
4. Langner, E., Deghani, H., El Hachemi, M., Belouettar-Mathis, E., Makradi, A., Wallmersperger, T., Gouttebroze, S., Preisig, H., Andersen, C. W., Shao, Q., Hu, H., Belouettar, S. "Physics-based and data-driven modelling and simulation of Solid Oxide Fuel Cells." International Journal of Hydrogen Energy 96 (2024): 962-983.
5. Semenov, A., Langner, E., El Hachemi, M., Belouettar, S., Wallmersperger, T. "Modelling and simulation of the electro-chemo-thermo-mechanical behaviour of solid oxide fuel cells considering creep". Acta Mechanica. 2025 (submitted).

Member in the network of: DRESDEN concept SCIENCE AND INNOVATION CAMPUS

Funded by: M-ERA.NET
SAB SÄCHSISCHE AUFBAUBANK
Luxembourg National Research Fund
Forskningsrådet