MEDIATE

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

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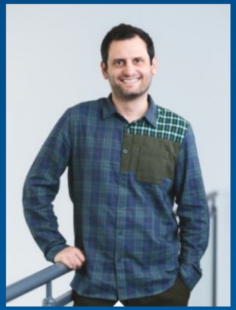
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1. Solid oxide fuel cells (SOFCs)
Motivation

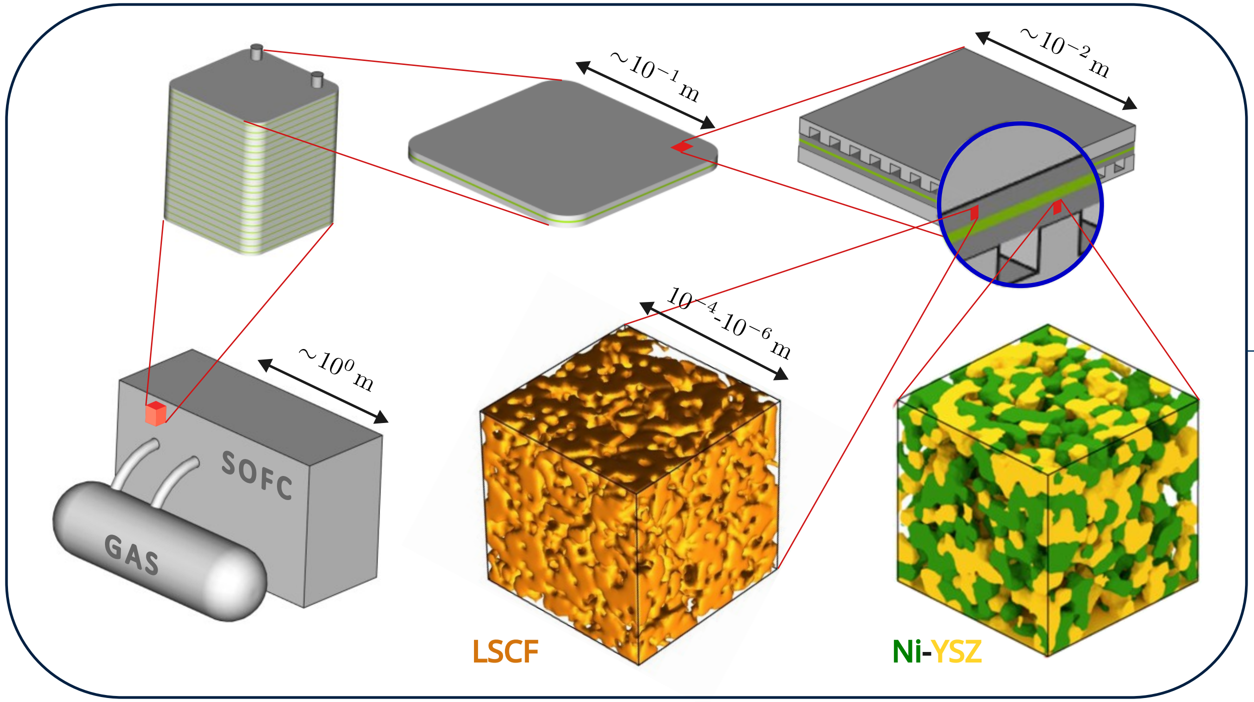
SOFCs:
- Direct conversion of chemical into electrical energy
- High energy efficiency (> 80%)
- Low environmental pollution

Redox reactions:

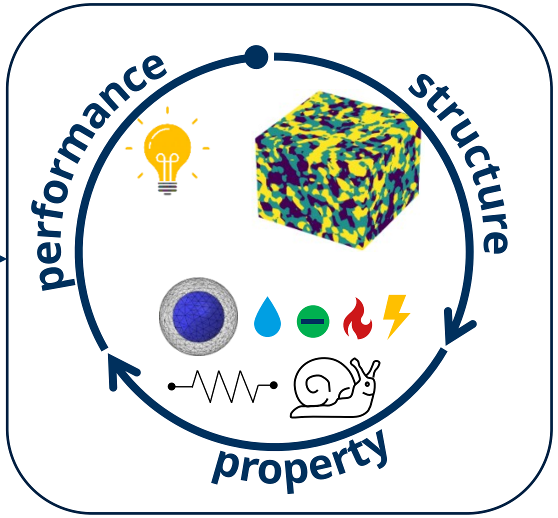
Cathode: $0.5\,O_2 + 2\,e^- \longrightarrow O^{2-}$

Anode: $H_2 + O^{2-} \longrightarrow H_2O + 2\,e^-$

SOFC analysis at different length scales

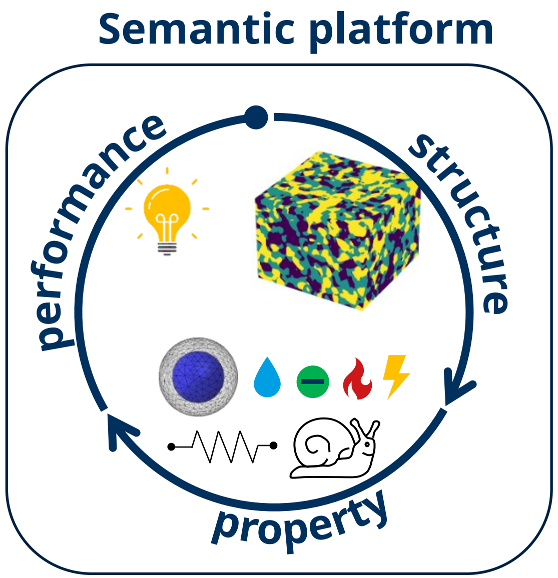


Semantic platform

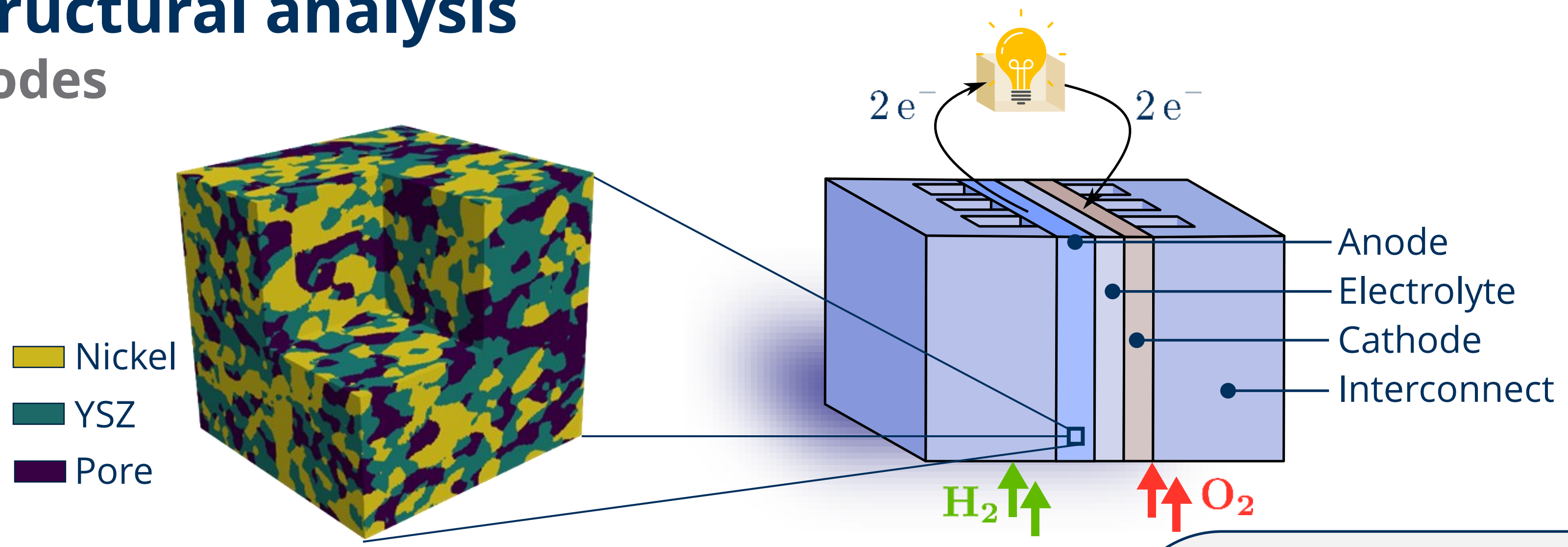


Outline

1. Motivation
2. Microstructural analysis
3. Macroscopic modeling
4. Semantic Platform
5. Conclusion and outlook



2. Microstructural analysis
SOFC electrodes



Geometrical parameters D

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

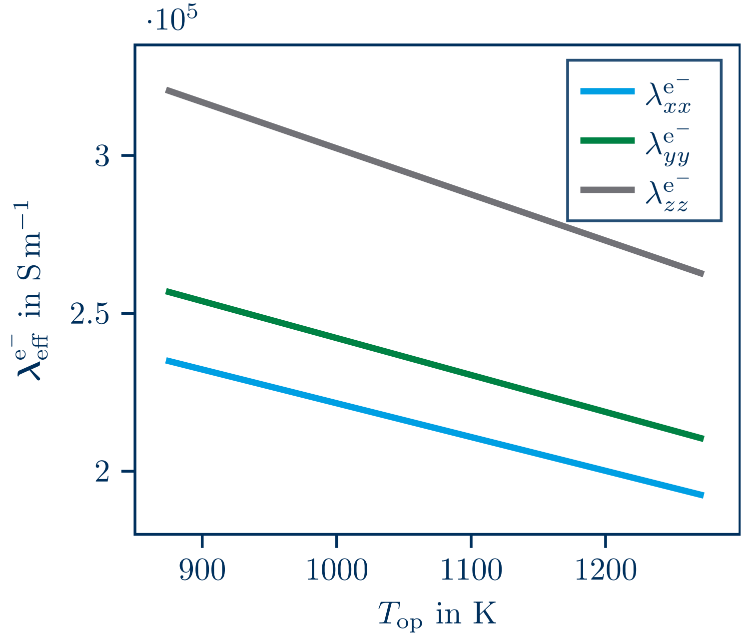
Computational homogenization →

Physical quantities

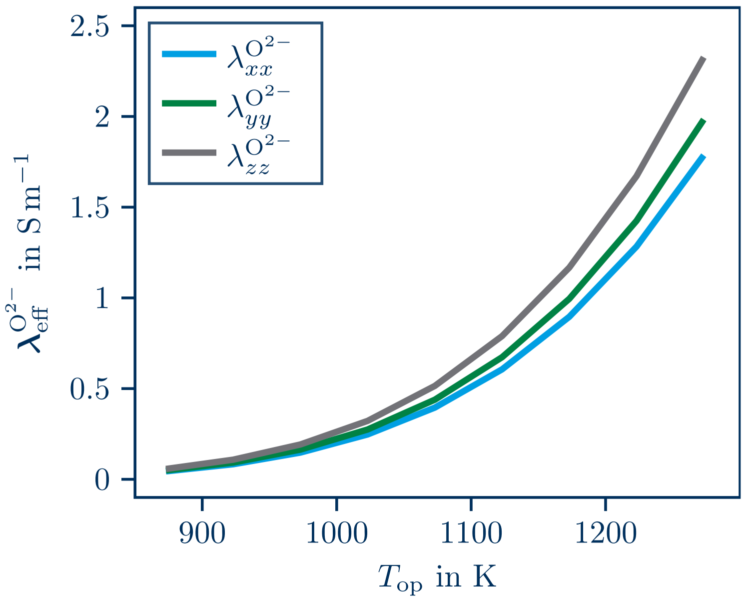
- Conductivities
  - Thermal
  - Electric
  - Ionic
- Fluid permeability
- Mechanical behavior
  - Stiffness
  - Thermal expansion
  - Creep

2. Microstructural analysis

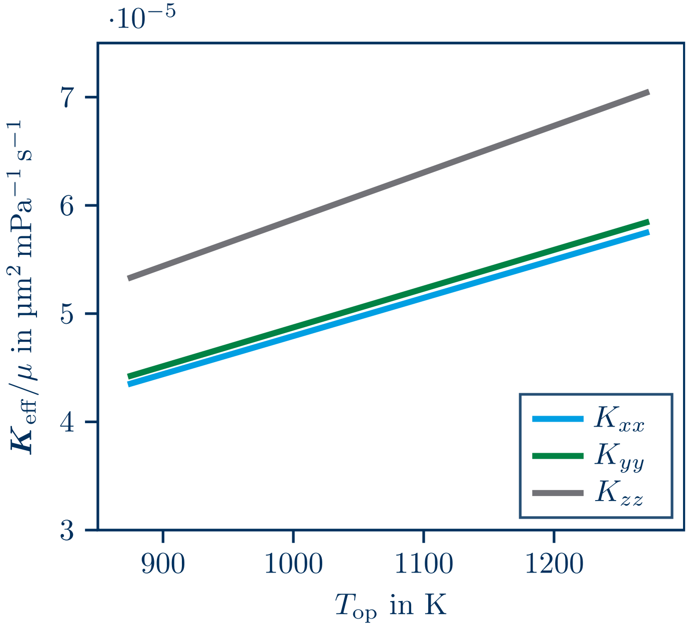
Effective properties: Transport [1]



Electric conductivity



Ionic conductivity



Permeability

[1] Langner et al., *PAMM*, 2024.

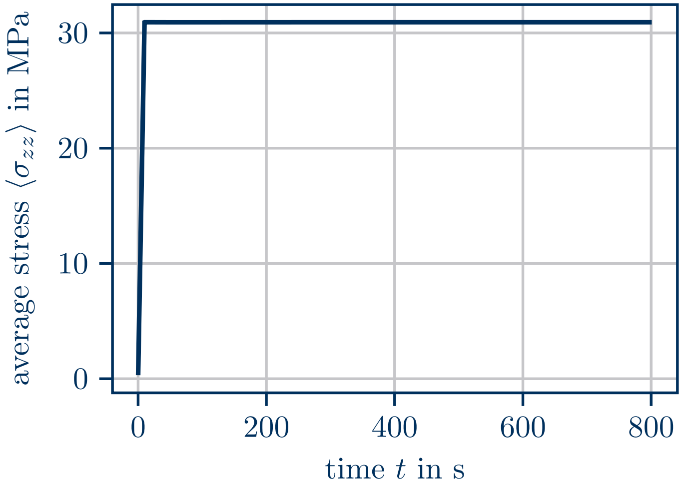
2. Microstructural analysis
Effective properties: Mechanics

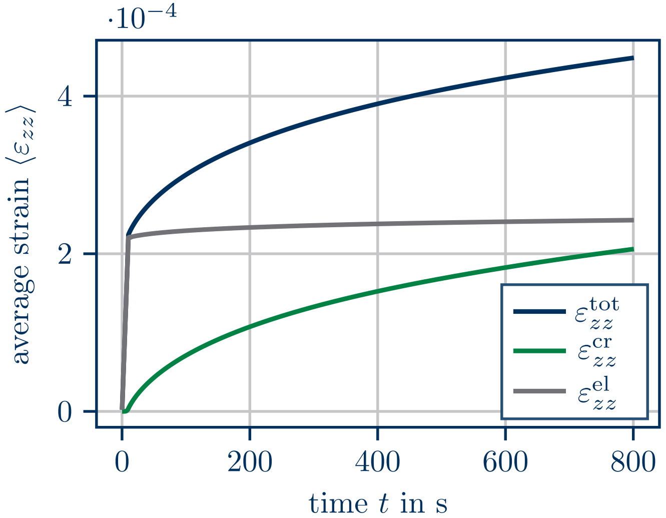
$$\nabla \cdot \boldsymbol{\sigma} = \mathbf{0}$$
$$\boldsymbol{\sigma} = \mathbb{C} : \boldsymbol{\varepsilon}^{\mathrm{el}}$$
$$\boldsymbol{\varepsilon}^{\mathrm{el}} = \boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{\mathrm{th}} - \boldsymbol{\varepsilon}^{\mathrm{cr}}$$

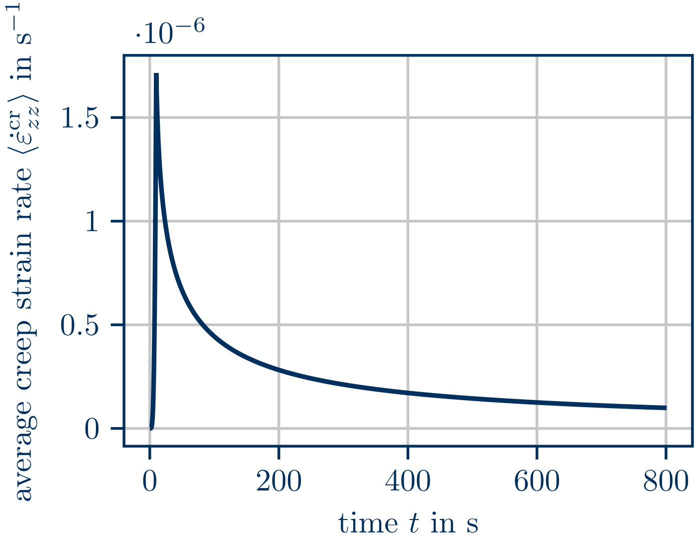
Norton model [2]: $Q = \frac{A}{n+1}\sigma_{\mathrm{eq}}^{n+1}$ with $\sigma_{\mathrm{eq}} = \sqrt{\boldsymbol{\sigma} : \mathbb{M} : \boldsymbol{\sigma}}$ →

$$\dot{\boldsymbol{\varepsilon}}^{\mathrm{cr}} = \frac{\partial Q}{\partial \boldsymbol{\sigma}} = A\sigma_{\mathrm{eq}}^{n-1}\mathbb{M} : \boldsymbol{\sigma}$$

Exemplary **load case *i*:** tension in *z*-direction







$$\mathcal{L} = \min_{A,n,G,F,L,M,N} \sum_i ||A\sigma_{\mathrm{eq}}^{n-1}\mathbb{M}(G,F,L,M,N) : \langle\sigma\rangle_i - \langle\dot{\boldsymbol{\varepsilon}}^{\mathrm{cr}}\rangle_i|| \longrightarrow A, n, G, F, L, M, N$$

[2] Norton, 1929.

2. Microstructural analysis

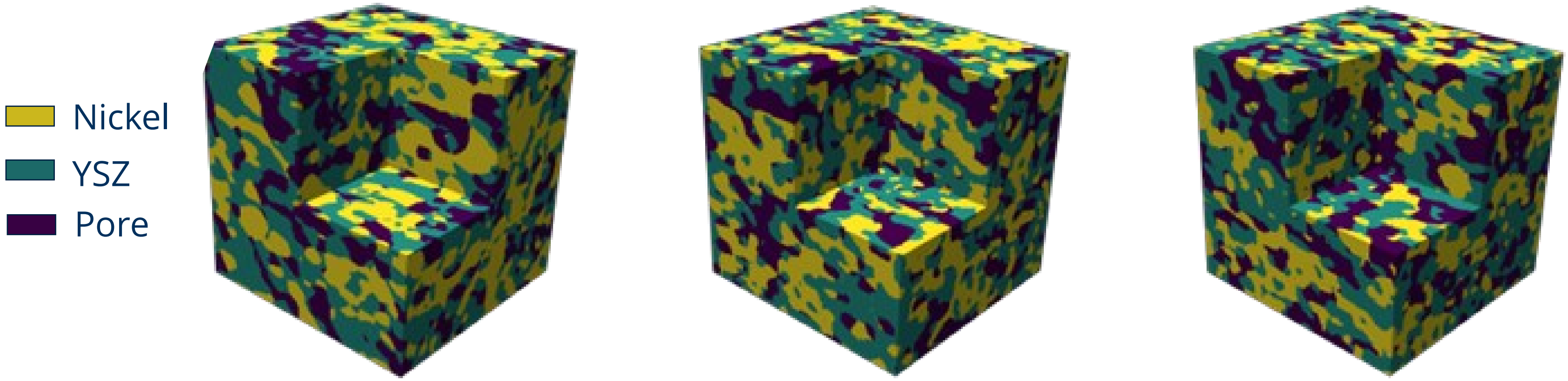
Reconstruction of anode microstructures*

$$M^{\text{rec}} = \underset{M}{\arg\min}\, \mathcal{L}\left(\{D_i(M), D_i^{\text{des}}\}_i^{n_D}\right)$$

$$\mathcal{L}(M) = \|D_i - D_i^{\text{des}}\|_{\text{MSE}}$$

	κ_{eff}	$\lambda_{\text{eff}}^{\text{e}^-}$	$\lambda_{\text{eff}}^{\text{O}^{2-}}$	$\alpha_{\text{eff}}^{\text{th}}$	K_{eff}	$\mathbb{C}_{\text{eff}}$
$\mathcal{E}^{\text{full}}$ in %	2.62	6.76	5.01	3.77	11.80	2.08
$\mathcal{E}^{\text{slices}}$ in %	6.67	8.99	10.36	6.87	14.17	3.25

$$\mathcal{E} = \frac{\|\bullet^{\text{rec}} - \bullet^{\text{orig}}\|_F}{\|\bullet^{\text{orig}}\|_F}$$



Original microstructure from FIB-SEM tomography [3] M^{orig}

Reconstructed microstructure based on full 3D tomography M^{full}

Reconstructed microstructure based on 3 orthogonal slices M^{slices}

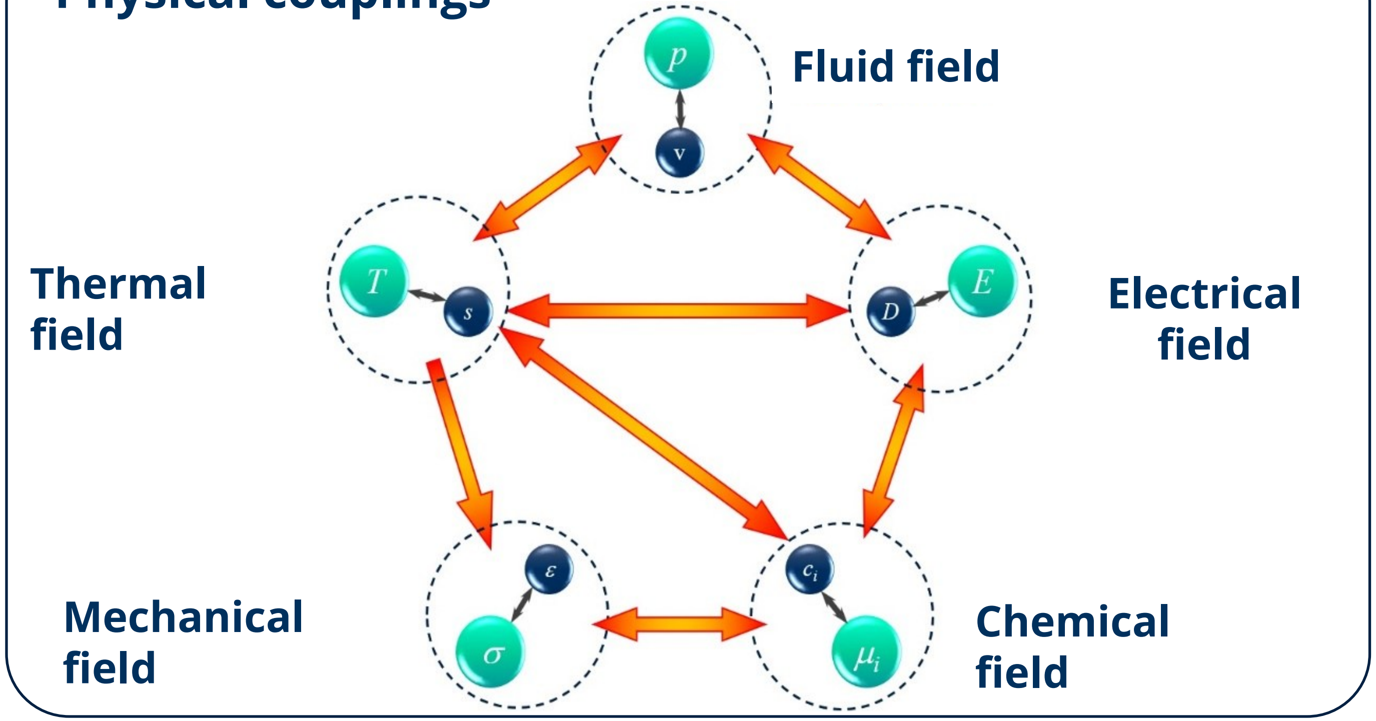
[3] Holzer et al., *Zenodo*, 2021.

* Collaboration with Seibert (TU Dresden)

3. Macroscopic modeling
Multiphysical problem [4,5,6]

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

Physical couplings

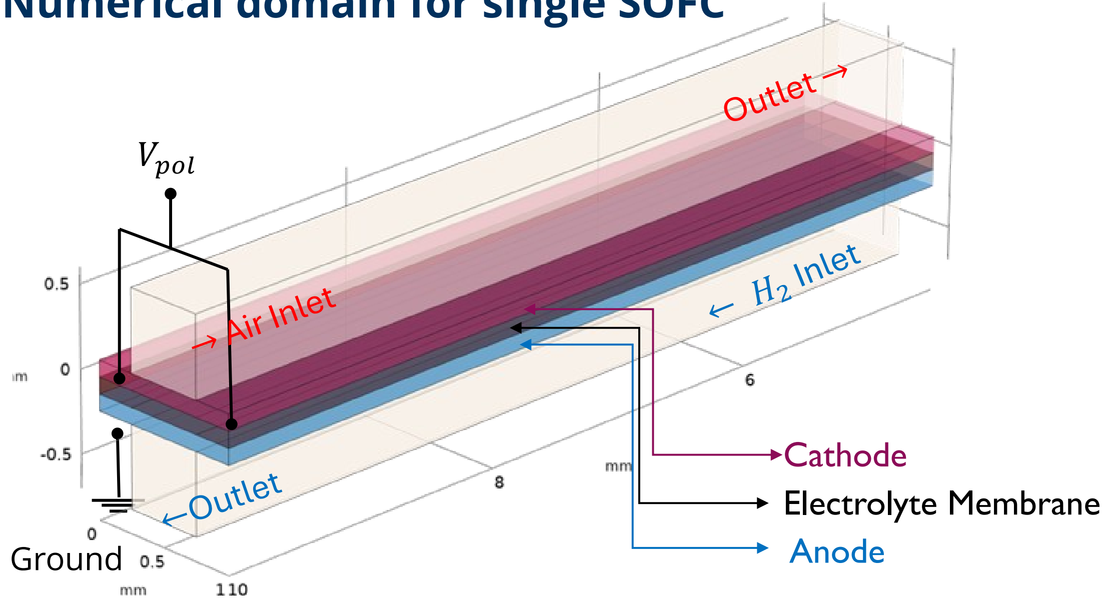


[4] Langner et al., *Int. J. Hydrog. Energy*, 2024.
[5] Belouettar et al., *Acta Mechanica*, 2025. *(submitted)*
[6] Semenov et al., *Acta Mechanica*, 2025. *(accepted for publication)*

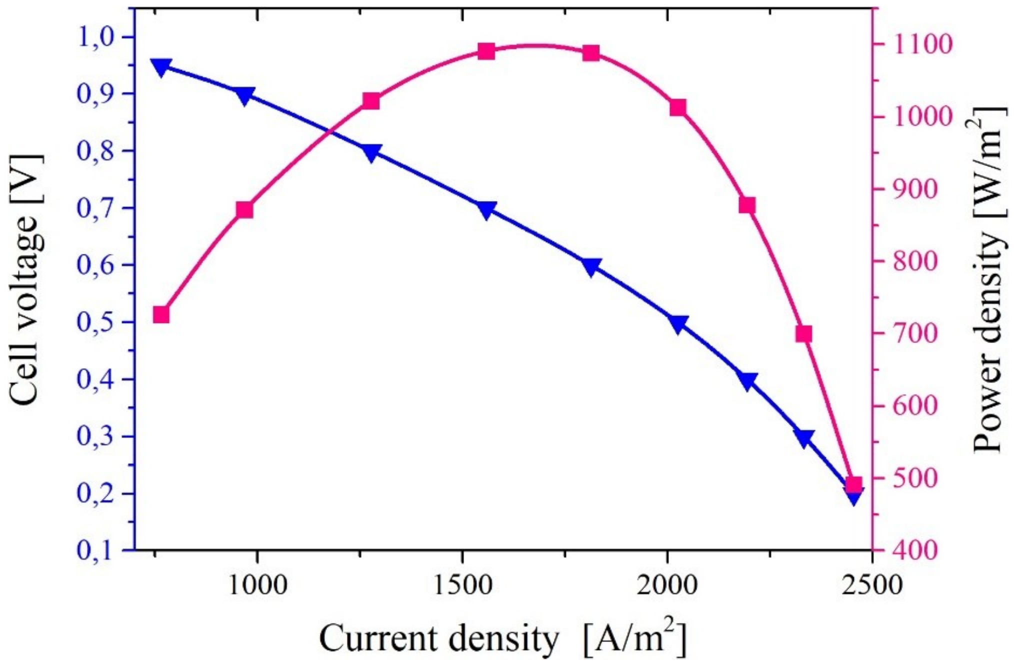
3. Macroscopic modeling

Results [5,6]

Numerical domain for single SOFC



SOFC efficiency



Cell voltage versus current density (blue)
Power density versus current density (pink)

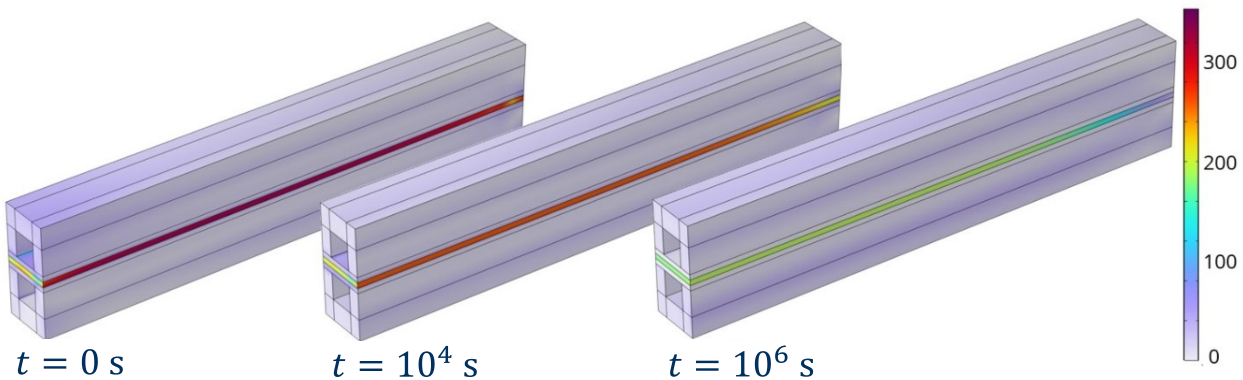
[5] Belouettar et al., *Acta Mechanica*, 2025. *(submitted)*

[6] Semenov et al., *Acta Mechanica*, 2025. *(accepted for publication)*

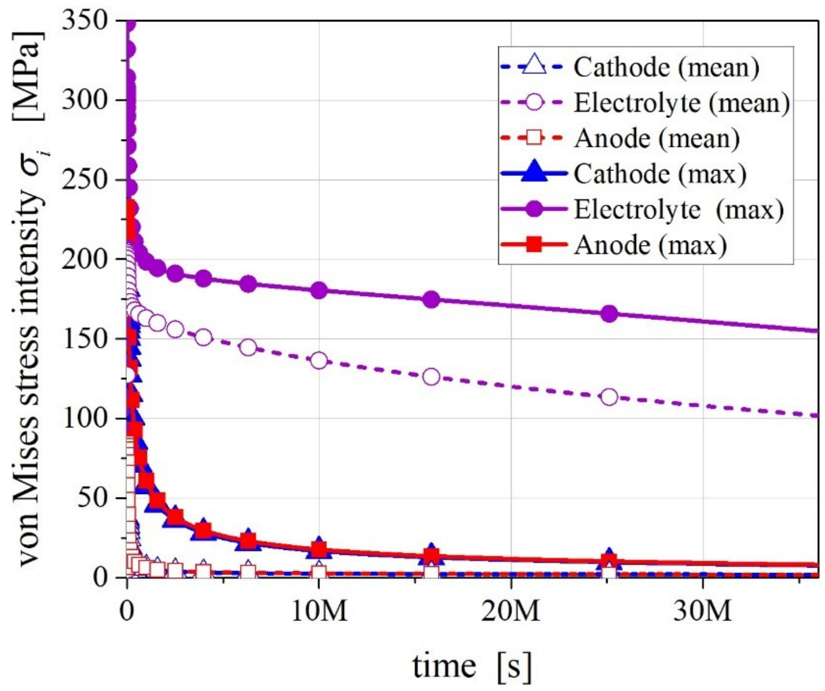
3. Macroscopic modeling

Results [6]

SOFC long-term durability



$t = 0$ s $t = 10^4$ s $t = 10^6$ s



Von Mises stress intensity versus time for the components of a single SOFC

[6] Semenov et al., *Acta Mechanica*, 2025. *(accepted for publication)*

3. Macroscopic modeling

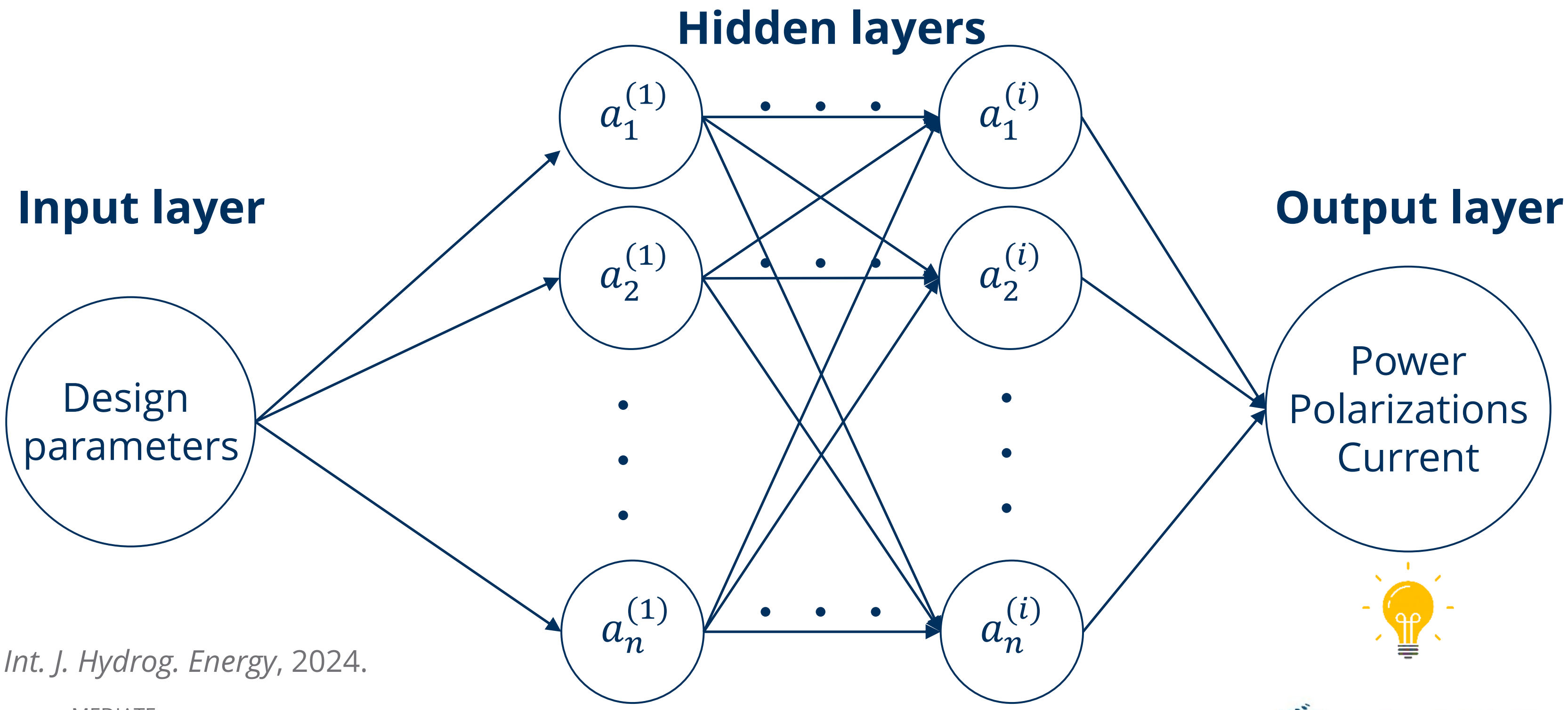
Surrogate model: Artificial Neural Network (ANN) [4]

Design parameters

- Geometrical parameters of single fuel cell
- Electrode properties
- Operating parameters

Optimization techniques for ANN

- Levenberg-Marquardt (LM): more effective for sparse datasets and smaller networks
- Adam optimizer: better performance for large datasets



[4] Langner et al., *Int. J. Hydrog. Energy*, 2024.

4. Semantic platform [4]

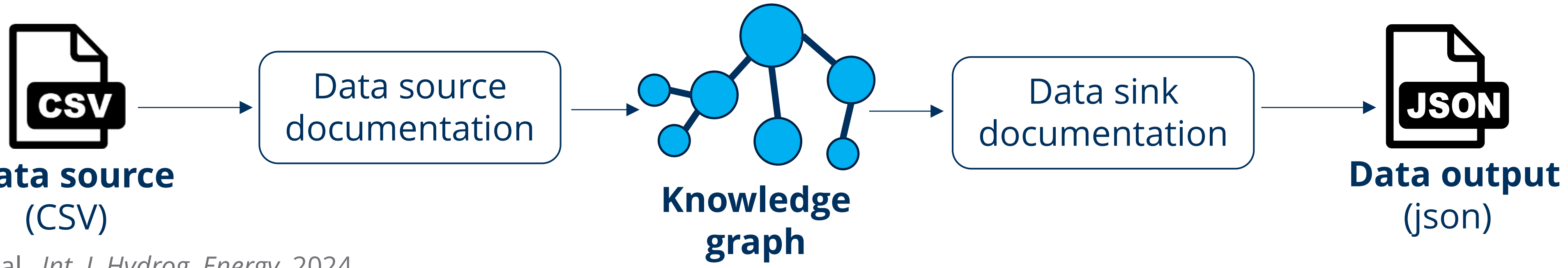
Structured ontology framework

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

Use of platform

- Connects multiphysical and multiscale models
- Organization of simulation data for reuse
- Reduction of inconsistences between data
- Improvement of data exchange and optimization of models

Example:



[4] Langner et al., *Int. J. Hydrog. Energy*, 2024.

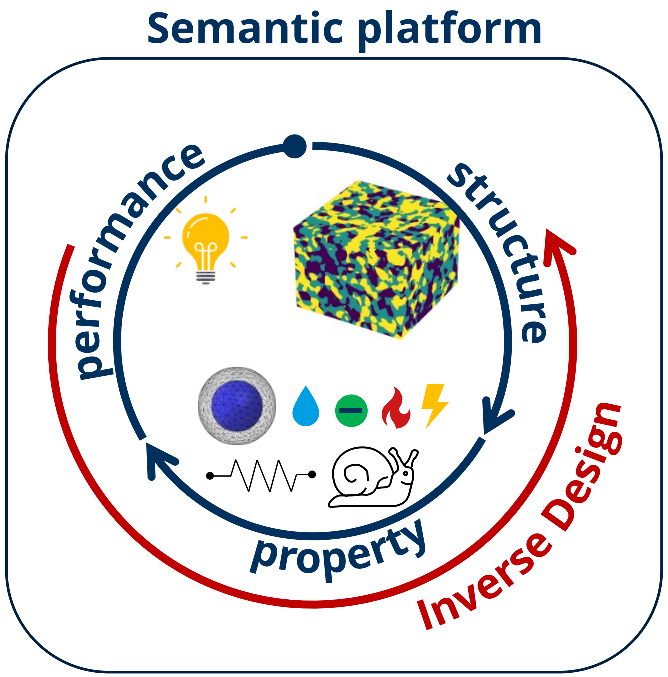
5. Conclusion and outlook

Conclusion

- Geometrical characterization of solid oxide fuel cell anodes
- Framework to determine effective properties
- Reconstruction of SOFC anodes
- Macroscopic modeling considering inelastic mechanical behaviour
- Surrogate modeling for fast predictions
- Integration into a semantic platform

Outlook

- Inverse design for electrode microstructures
- Further implementation of structure-property-performance relationships into the platform
- Inclusion of manufacturing process into the framework
- Optimization of SOFC to maximize performance and long-term durability
- Validation and comparison with experimental data



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References

[1] 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.

[2] Norton, F.H. "The Creep of Steel at High Temperatures". McGraw-Hill Book Company, New York. 1929.

[3] Holzer, L., Pecho, O., Hocker, T., Iwanschitz, B., Mai, A. (2020). "FIB-tomography data of Ni-YSZ anodes for Solid Oxide Fuel Cells (SOFC): Comparison of pristine and degraded materials (before/after redox cycling)" (Version 1) [Data set]. Zenodo. 2021.

[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] Belouettar, S., 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)*

[6] 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). *(accepted for publication)*