

Numerical model reduction of the electro-chemically coupled ion transport

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ABSTRACT

This contribution concerns the multi-scale and multi-physics Finite Element Analysis of the electro-chemically coupled ion transport^[1]. In particular, we are interested in predicting the electro-chemical performance of the Structural Battery Electrolyte (SBE) by utilizing computational homogenization and numerical model reduction^[2] (NMR).

A sub-scale Representative Volume Element (RVE) is generated for the two-scale modeling approach. It represents the random bicontinuous microstructure of an SBE (porous polymer skeleton filled with liquid electrolyte).

The governing equations consist of Gauss' law, mass balance of the pertinent ions and linear constitutive relations. Periodic boundary conditions are imposed on the RVE according to first order homogenization on the electrical and the chemical potential fields. The fully coupled electro-chemical problem is solved to obtain the macroscopic (homogenized) transient response. By solving the RVE problem for various loading cases, we obtain training data that are used for NMR based on a snapshot Proper Orthogonal Decomposition (POD).

The end product of the NMR-POD framework is a surrogate model which replaces RVE computations. Since the surrogate model consists of a system of ODEs, it requires less computational effort to solve compared to the full RVE problem. The final goal is to investigate how the choice of training data and POD modes affect the simulation accuracy, and also quantify the speed-up by exploiting the surrogate model.

REFERENCES

- [1] Tu, V., Larsson, F., Runesson, K. and Jänicke, R. Variationally consistent homogenization of electrochemical ion transport in a porous structural battery electrolyte. *Eur. J. Mech. A Solids* (2023) **98**:104901.
- [2] Jänicke, R., Larsson, F. and Runesson, K. A poro-viscoelastic substitute model of fine-scale poroelasticity obtained from homogenization and numerical model reduction. *Comput. Mech* (2020) **65**:1063–1083.