Numerical model reduction of the electro-chemically coupled multi-scale transport of electroactive species

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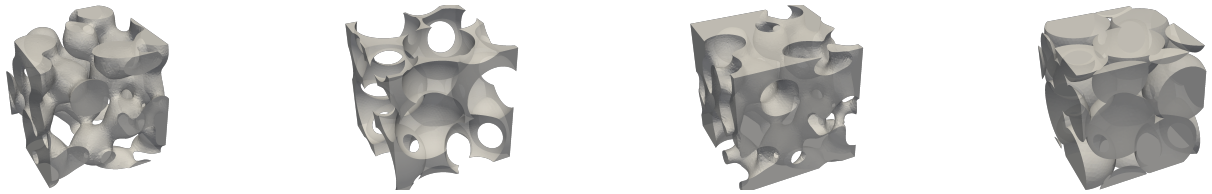
ABSTRACT

Carbon fibers are mostly used as structural reinforcement materials, but they can also serve as high capacity Li-ion battery negative electrodes. By utilizing the carbon fiber's intrinsic ability to carry load and to insert lithium ions, a new type of multi-functional material called the structural battery composite can be realized.[1]

The focus of this presentation is on the multi-scale and multi-physics Finite Element Analysis of the structural battery composite. We are particularly interested in predicting the electro-chemical performance of the Structural Battery Electrolyte (SBE) by utilizing computational homogenization,[2] and numerical model reduction (NMR).[3]

For our two-scale modeling approach, we numerically generate sub-scale Representative Volume Elements (RVE) representing the stochastic bicontinuous microstructure of an SBE (porous polymer skeleton filled with liquid electrolyte), see Figure 1.



(a) (b) (c) (d)

Figure 1: Numerically generated 3D RVEs with various shapes and porosities.

We impose periodic boundary conditions on the RVE according to first order homogenization on the electrical and the chemical potential, and then solve the fully coupled electro-chemical problem to obtain the macroscopic (homogenized) transient material response via volume averaging. By exploiting NMR based on a snapshot Proper Orthogonal Decomposition (POD), we aim to simulate the SBE's electro-chemical performance on the macro-scale.

Lastly, since the NMR results in a surrogate model that requires a training phase, we also investigate how the choice of training load cases and POD modes affects the simulation accuracy.

REFERENCES

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