

Machine learning strategies to predict ion transport through a porous Structural Battery Electrolyte

Background

One major challenge on the way towards a carbon-neutral circular economy is to find innovative solutions for a light-weight storage of electric energy. This need gives rise to the development of structural battery composites that combine the functionalities of bearing mechanical loads and storing electric energy in the same device.

Goal

The goal of this thesis project is to use Deep Neural Networks (DNN) to predict ion transport through a porous Structural Battery Electrode (SBE). The SBE consists of a polymer matrix, the pore space is filled with an ion-conducting liquid electrolyte, see Fig. 1. Ion transport takes place via two different mechanisms: i) diffusion driven by a concentration gradient, ii) convection. Here, convection means that the electrolyte itself is flowing through the pore space, e.g. driven by a compression of the structure. In this thesis project, linear (Fickian) diffusion and linear Stokes flow will be used to simulate those two contributions to the ion transport. The overarching goal is to train a DNN with data stemming from simulation of diffusion and Stokes flow through synthetic 2D/3D SBE structures, see Fig. 2. The trained DNN shall be able to predict homogenized properties (ionic conductivity, permeability) for unknown SBE structures.

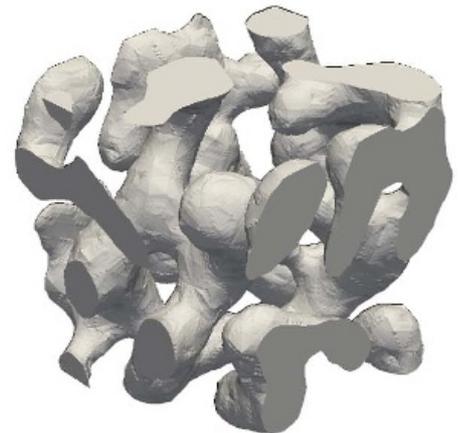


Figure 1: Synthetic SBE structure

Your tasks in this project will be:

- Generation of synthetic (i.e. for computer simulation) Representative Volume Elements (RVE) of SBE structures
- Simulation of ion transport to obtain training and validation data
- Design and training of a DNN in Keras/TensorFlow

Main steps in the project

- Literature study, theoretical background
- Generation of synthetic SBE structures, simulation of transport properties
- Implement and train DNN, validate network

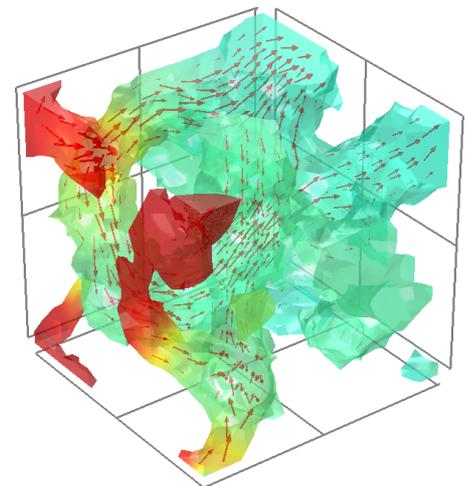


Figure 2: Simulation of Stokes flow through a synthetic SBE

Student background

This project is preferably suitable for students with an interest in computational mechanics and the finite element method. The project will give you an understanding in multi-physics modeling and FE simulation. At the same time, the project and its result will be part of current research at the Division of Material and Computational Mechanics.

Conditions: The thesis work comprises 30 ECTS and will be conducted during January-June 2021. The project is suitable for individual students or for teams of 2 students.

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