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.

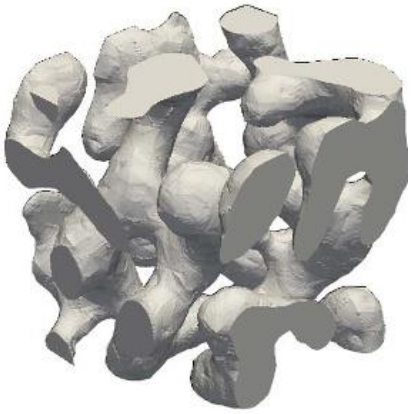

Figure 1: Synthetic SBE structure

Tasks

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

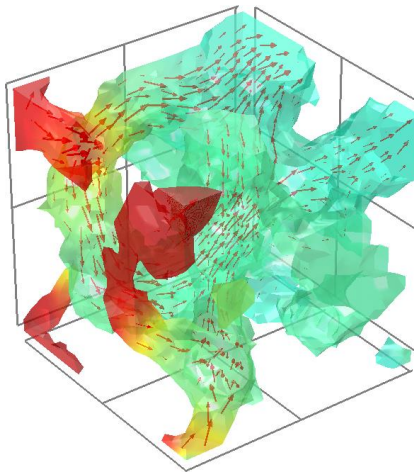

Figure 2: Simulation of Stokes flow through a synthetic SBE

Main steps in the project

The following main steps will be taken in this project.

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

Student background

This project is suitable for one or preferably two students with an interest in computational physics and the finite element method. Programming skills are highly valued, and previous experiences with finite element analysis is a plus. The project will give you an understanding in multi-physics modeling and FE simulations. At the same time, the project and its result will be part of an ongoing research at the Division of Material and Computational Mechanics at Chalmers.

Supervisors:

Mohsen Mirkhalaf, University of Gothenburg, mohsen.mirkhalaf@physics.gu.se
Ralf Jänicke, Chalmers University of Technology, ralf.janicke@chalmers.se

UNIVERSITY OF GOTHENBURG

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