



A chemo-mechanical multi-scale model for the application of numerical model reduction

To make predictions for engineering applications, simulations of the physical behavior of a system are a valuable tool. In this context, multi-scale modeling allows the simulation of a system accounting for properties of the materials micro-structure.

In a so called FE^2 -setting, a homogeneous material is considered at the macro-scale while the micro-structure is represented by a Representative Volume Element (RVE). Then, for every quadrature point at the macro-scale, a boundary value problem on the RVE is solved to obtain the effective material properties. This reduces the cost of one huge problem to multiple smaller problems, however, the often large number of RVE problems still makes this procedure computationally expensive.

For this reason, techniques to speed up the computation of the RVE problem are required. One such a technique is Numerical Model Reduction (NMR) via snapshot Proper Orthogonal Decomposition (POD), where the complete solution is split into a set of modes. This way, the partial differential equation(s) with many degrees of freedom is replaced by a set of ordinary differential equations with way fewer degrees of freedom.

In this project, we aim to implement a (linear transient) chemo-mechanical multi-scale model (cf. [1]), which is equivalent to poro-elasticity, and prepare it for the application of NMR (cf. [2]) using Ferrite.jl. The project has following main steps:

- Implementing the (linear) chemo-mechanical multi-scale model
- Testing the implementation for some examples
- Preparing the RVE problem for NMR via snapshot POD

As outcome of the project, three main components are expected:

- A short report with the mathematical model and some numerical results
- The implementation of the model (as a Julia module)
- A proper documentation of the code

References

- [1] David Rene Rollin et al. “Upscaling of chemo-mechanical properties of battery electrode material”. In: *International Journal of Solids and Structures* 281 (2023), p. 112405. DOI: 10.1016/j.ijsolstr.2023.112405.
- [2] Ralf Jänicke et al. “A poro-viscoelastic substitute model of fine-scale poroelasticity obtained from homogenization and numerical model reduction”. In: *Computational Mechanics* (2020). DOI: 10.1007/s00466-019-01808-x.

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