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# NUMERICAL HOMOGENIZATION AND MODEL REDUCTION FOR TRANSIENT HEAT, DIFFUSION AND COUPLED MECHANICS PROBLEMS

This dissertation presents computationally efficient numerical homogenization techniques for transient diffusion phenomena in heterogeneous materials. The transient behavior arises due to the material properties, the characteristic length scales and the time varying loading conditions. Homogenization of such materials generally requires computationally expensive solution schemes for the transient diffusion equations at the macro-and the micro-scale. Concepts from numerical techniques like computational homogenization, component mode synthesis and data-driven mechanics are used to efficiently homogenize problems for heat diffusion, mass diffusion and mass diffusion coupled to mechanics. The background and motivation is presented in Chapter 1.

In Chapter 2, as a preliminary step, a model reduction for the transient heat diffusion equation is performed at the micro-scale using component mode synthesis, which provides an emergent enriched-continuum description of the homogenized level at the macro-scale. Assuming linear material behavior and relaxed separation of scales, the microscopic response is decomposed into a steady-state and a transient part. For the steady-state response static-condensation is used, whereas for the model reduction of the transient response an eigenvalue problem is solved and the system of equations is projected onto a reduced number of eigenbases. As a consequence, the microscopic problem is replaced by a set of decoupled ordinary differential equations which are computationally inexpensive to solve. The numerical examples solved at the micro-scale confirm the accuracy and computational efficiency of the method.

Chapter 3 deals with different solution methods for the macro-scale enrichedcontinuum for transient mass diffusion problems. Two spatial discretization schemes are discussed for the enrichment-variables. The primary macroscopic field is interpolated with finite element shape functions, while the enrichment-variables can either be interpolated using finite elements, leading to a multi-field solution method, or evaluated at the Gauss quadrature points, leading to an internal-variable solution method. Different time integration methods are also presented for the internal-variable solution method. Enriched-continuum results are compared with those obtained from classical transient homogenization and direct numerical simulations for evaluating the accuracy and computational gains.

The proposed model reduction method is extended to the transient mass diffusion coupled to the mechanics, in Chapter 4, with application to lithium-ion batteries operating in a linear regime. Using the Legendre transformation, the primary variables of the coupled model are converted to the chemical potential and strain fields, which allows the use of standard C0-continuous finite elements. A model reduction using component mode synthesis is performed and an enriched-continuum for mass diffusion coupled to mechanics is obtained. The micro-scale problem, which usually involves an expensive solution of the coupled mass diffusion-mechanics problem, is now replaced by a set of ordinary differential equations.

Chapter 5 constitutes a novel model reduction and homogenization procedure for history dependent diffusion at the macro-scale using data-driven mechanics. It replaces the solution of the microscopic problems with a direct search in a data-set. The data-set is generated efficiently using the enriched-continuum formulation in an offline stage. The enrichment-variables serve as a pointer in time for keeping track of the history dependent diffusion. It also provides a route to extend the proposed model reduction method to the non-linear regime. Finally, conclusions and future research directions are discussed in Chapter 6.

Mots-clés : computational homogenization, model order reduction, non-fickian diffusion, data-driven mechanics