Enriched Continuum Formulation based on Computational Homogenization for Transient Diffusion Problems.

A. Waseem†, T. Heuzé†, L. Stainier†, M.G.D. Geers† and V.G. Kouznetsova†

† Department of Mechanical Engineering, Eindhoven University of Technology, 5600 MB Eindhoven, The Netherlands

‡ Institut de Recherche en Génie Civil et Mécanique, GeM, UMR 6183 - CNRS - École Centrale de Nantes, France

ABSTRACT

Transient diffusion problems with high contrast in material properties and rapidly varying loading conditions exhibit inertial effects at the microscale e.g., mass diffusion in batteries and fuel cells. Computational homogenization (CH) has proven to be a reliable method to solve quasi-static [1], steady-state [2] and also transient [3, 4] problems for heterogeneous materials in a multi-scale setting. For linear problems, CH essentially consists in the construction of effective constitutive tensors from the micro-scale model, usually taken as a representative volume element. In contrast to static and steady-state problems, analysis of transient problems with non-negligible micro inertia effects necessitates to evaluate the effective constitutive tensors at each macroscopic material point for each time increment, which makes it quite expensive.

In this work, a computationally tractable procedure is developed for computational homogenization of transient diffusion problems, which can accurately capture the inertial effects at the microscale. First, the weak separation of scales [4] is identified for a transient diffusion problem and for the linear material model the micro-scale solution is decomposed into steady-state and transient responses. Then, a reduced basis is sought using static condensation and eigenvalue analysis of the representative microscopic unit cell, allowing to express the macroscopic constitutive tensors in terms of this reduced basis. This gives rise to an enriched continuum description at the macro-scale featuring the coefficients of the reduced basis as enriched fields, for which the evolution equations naturally emerges to be solved together with the mass balance equation. Compared to the conventional transient homogenization it replaces the microscopic problem with a set of decoupled ordinary differential equations, which saves computational effort.

Several solution procedures, based on different spatial and temporal discretization schemes, are proposed for enriched continuum. Proof-of-principle simulations are conducted using Li-ion cathode-electrolyte system. Significant gains in computational times are observed without loss of accuracy.

REFERENCES


