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Titre de thèse : Numerical Modeling Strategy for Heterogeneous Materials: A FE Multi-scale and Component-based Approach

Mots-clefs : heterogeneous materials, multiscale modeling, code coupling, software component technology.

Résume :

Many industrial applications rely on the a priori knowledge of a given set of parameters assumed to characterize expected observable and macroscopic behaviors or properties. In mechanical and civil engineering, during the structure design process { from aircraft wing to bridge platform { the service and ultimate bearing capacities are computed assuming material parameters which govern their constitutive material behavior laws. The better the latter are known, the more optimized structures can be. Hence, an old though still current research area is to seek relevant material models in order to design both reliable and economical structures and tailor new composite materials, in order to fulfill the weakness of one material with the strength of others.
The first material mechanical models only rely on macroscopic observations which were the only available pieces of information. Thanks to more and more sophisticated investigation techniques meso, micro, even nano scale observations are accessible. Scanning Electron Microscope (SEM) or Transmission Electron Microscope (TEM) allow 2D images of material inner structure to be captured. X-ray tomography allows to access directly the 3D structure of tested specimen. All these fine scale observations unveil the heterogeneous character of most materials. A current challenge is, thus, to incorporate all these details in material models.
The goal is to trigger phenomena on their scale of occurrence using refined models. For instance, regarding concrete, air voids have approximately 1mm radius and are known to have an important role [Yaman et al., 2002] in the failure process. Deriving macroscopic laws on a representative volume element, macroscopic models cannot account for these different scales. Hence, there is a call for a framework capable of gathering mechanical phenomena described on their pertinent scale as well as bringing them on the structural level. Numerical simulations may present a method to meet this goal.
Together with the increase optical device resolution, computational power has tremendously risen in the past five decades. Dealing with Finite Element method, a lot have been achieved from the thousand degrees of freedom (DOF) solved on dam problems in the early sixties [Clough, 1960] to the half billion DOF of the Gordon Bell prize 2004 [Adams et al., 2004]. Thus, the current trend is to explicitly model heterogeneous micro structures in Finite Element computations in order to bring as much physical data as possible into numerical models. Indeed, these models require a large number of DOF and call for dedicated numerical tools.
The aim of such refined computations should be to bring on a coarser and more relevant scale pieces of information detailed enough to allow more accurate structural designs. This up-scaling process is often referred to as homogenization. The present dissertation is concerned with the development of numerical homogenization tools which may be divided into two groups following

[Feyel and Chaboche, 2001]. Sequential approaches tend to build macroscopic models from a sequence of lower scale computations. Most of them rely on a probabilistic description of phases arrangement or material properties on the fine scale. The incomplete knowledge of phenomena motivates the use of random models and the computation sequence often referred to as Monte Carlo integration [Caisch, 1998]. Assuming ergodicity, the spatial averages and higher order moments are used to find both effective properties {intrinsic to the material and not to the specimen size {and their related Representative Volume Element (RVE) { [Kanit et al., 2003], [Lachihab and Sab, 2005]. On the other hand, integrated approaches carry out macro computations enriched by finer scale ones. Most of them are based on the Finite Element method and on an explicit communication between the coarse and the fine grid: through Gauss points [Feyel and Chaboche, 2000] or gluing areas [Ben Dhia, 1998]. In the present work, the integrated approach is preferred. Both the theoretical formulation and the implementation of an original strategy are discussed herein. The latter is dedicated to model materials for which the scale separation may not hold. Cement based materials are of this kind, the characteristic lengths of different heterogeneities between two scales of observation is not typically small enough to consider these levels as entirely separated. For instance, classic compression tests are performed on concrete cylindrical specimens of 16cm diameter and 32cm height and the size of aggregates is typically 1 or 2cm. Obviously, the specimen scale and the aggregate scale are strongly coupled.

From a quite different point of view, the proposed approach takes after the Finite Element design with embedded kinematics. The pursued idea is to build up a refined description within each element of the structural discretization in order to provide an enriched upscaled behavior. Thus, in desired areas of a structure, macro elements may be seen as micro models containers provided with their own discretization. Localized Lagrange multipliers [Park et al., 2000] hook up together the two description levels. Hence, the proposed method borrows some features from the non-overlapping domain decomposition strategies [Gosselet and Rey, 2006]. Still, since the aim of the method is to build up an enriched macroscopic description from microscopic ones, it cannot actually be considered as a domain decomposition strategy. The first chapter of the dissertation covers these theoretical details. Common tools that have been set up in the domain decomposition literature are reintroduced. Moreover, integrated multi-scale strategies are reviewed. It is shown how some domain framework, MuSCAd { Multi-Scale Strongly Coupled Algorithm Component Architecture { has, thus, been developed in a particular programming context, the component oriented paradigm [Szyperski, 1998]. It extends the notion of class to independent pieces of software, namely components, able to communicate and interoperate over a computer network. This quite recent technology also enables to integrate existing codes and libraries in more general frameworks. Parallel invocations and executions are natural features of component software. It also offers the possibility to develop general frameworks and different components can be exchanged as long as they fit in with the same specifications. Hence, the MuSCAd framework uses, on the micro level, a component from the Finite Element program FEAP [Taylor, 2008] which may be replaced by any other FE code.

The second chapter addresses the implementation of the method. Each specificities are detailed for each computational level { the macro level, the boundary one and the micro one. A software framework realization implies choices that are, each time, motivated and discussed. Academic examples are presented to validate and present the framework capabilities in terms of convergence and computational cost { both CPU time and RAM requirements.

One of the most important goals which is aimed at in this dissertation is to show how the multi-scale framework MuSCAd is a relevant and useful tool to model the mechanical behaviors of the concrete and more generally cement based materials. Such materials are heterogeneous and exhibit brittle or quasi-brittle failure process that is a major point in computing the ultimate bearing capacities civil of engineering structures. Actually, the concrete structures collapse because of micro cracks merging into a macro ones. These two stages trigger an asymmetric response in traction and compression of concrete specimen and are hard to comprehend physically without a proper microscopic description. Thus, the third chapter is dedicated to testing the proposed integrated strategy as a tool for a concrete meso model developed at the LMT Cachan [Benkemoun et al., 2009]. Based on a lattice representation, it provides an explicit representation of heterogeneities and models the main features of quasi-brittle material failure process. After a detailed presentation of its capabilities, the last chapter discuss the first results obtained when it is coupled with the MuSCAd framework.

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5. Hautefeuille M., S. Melnyk, J.B. Colliat, A. Ibrahimbegovic, ‘Probabilistic aspects of localized failure of massive heterogeneous structures’, International Journal of Engineering Computations, 26, 166-184 (2009)

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6. M. Hautefeuille, J.B. Colliat, A. Ibrahimbegovic, H. Matthies, ‘Multi-scale strategy for heterogeneous materials with localized failure’, ECCM-2010 Fourth European Conference on Computational Mechanics (Solids, Structures and Coupled Problems in Engineering), Paris, France, May 16-21, 2010

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Plane Crash with Explosions, Fires, Wind Storms, Earthquakes with Tsunamis', Workshop on Construction under Exceptional Condition, Hanoi, Vietnam, October 29-31, 2010