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Distributed computing for the nonlinear analysis of multiphase composites

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Dedicated to Professor Zdeněk Bittnar in ocassion of his 70th birthday.

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ABSTRACT

Modern digital material approaches for the simulation and visualization of heterogeneous materials allow to investigate the behavior of complex multiphase materials with their physical nonlinear material response at various scales. However, these computational techniques require extensive hardware resources with respect to computing power and main memory to solve numerically large-scale discretized models in 3D. Due to a very high number of degrees of freedom, which may rapidly be increased to several 10 million degrees of freedom, the limited hardware resources are to be utilized in a most efficient way to enable an execution of the numerical algorithms in minimal computation time. The computational efficiency and the distribution among available hardware resources (often based on a parallel hardware architecture) can significantly be improved. In the past years, high-performance computing (HPC) based computation techniques were established for the investigation of scientific objectives. Their application results in the modification of existing and the development of new computational methods for the numerical implementation, which enables to take advantage of massively clustered computer hardware resources. Due to the high numerical effort for such simulations, an alternative approach for the nonlinear finite element analysis, based on the sequential linear analysis, was implemented in respect to scalable HPC. The incremental-iterative procedure in finite element analysis (FEA) during the nonlinear step was then replaced by a sequence of linear FE analysis, known in literature as saw-tooth approach. As a result, qualitative (smeared) crack initiation in 3D multiphase specimens has efficiently been simulated.

1. Introduction

The life-time assessment of engineering structures relies on sophisticated material models, integrating all different aspects of damage initiation and deterioration over the expected life-time of a structure. Therefore, the current material models in engineering applications are integrating modern approaches from material science via multiscale methods. Especially for heterogeneous materials, these multiscale approaches allow a detailed insight into the material physics on appropriate scales [10]. In (material) engineering science, the investigation of 3D material behavior, such as e.g. the damage initiation and propagation at different scales, is based on complex simulation models, which may require extensive computer resources, if they capture the heterogeneous nature and also include the specific material behavior of each material phase. By this, they are able to represent the damage behavior of the quasi-brittle material (such as concrete or mortar mixtures as complex matrix-inclusion based composites) up to the macroscale, where the damage is induced by accumulated effects of micro-cracking. In general, a major drawback of using multiscale methods is the tremendous increase in degrees of freedom (d.o.f.s.) of the resulting equation systems when studying models at micro- or mesoscale. In damage simulations, the incremental-iterative approach requires the repeated solution of the linearized equation system, resulting in an even more crucial computing time consumption.

The 'close to reality description' of the material behavior of multiphase composites at sub-macroscale (under specific boundary and loading conditions) is associated with the characterization of very complex physical processes, not only in the state of damage and collapse, but also in the initial configuration. There, different material phases are connected over a small interfacial transition zone (ITZ), which is dedicated to be the weakest link and therefore, the beginning of the initiation of (micro-) cracks and their accumulation and propagation to and through other phases, which often results in macroscale failure in materials and consequently, in the entire engineering structure. At a first step the phenomenological description of physical processes in 3D should be limited to the representation of mechanical degradation effects and, hence, microscale models with a spatial high resolution of the ITZ are considered. The type of material law considered for the phenomenological model of the ITZ is essential for a representation of the

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close to reality damage effects in multiphase materials. Here, the phenomenological model is often based on observed physical characteristics quantified in corresponding material properties and the resulting mathematical description of the physical (mechanical) problem results in partial differential equations (PDEs). The finite element method (FEM, [3]) as a standard discretization technique can be applied to solve such system of PDEs numerically, similar to the analysis of mechanical problems at the macroscale. In this paper, combined (hybrid) approaches for the suitable discretization, the efficient solution and the sophisticated representation of damage effects in multiphase materials are addressed. The main content is the investigation of a general hybrid discretization technique for three-phase materials and a distributed solution strategy adapted for the final system of equations. This hybrid discretization considers a volumetric ITZ in high-resolution around the inclusions, which are embedded in a regular grid. Due to the high numerical effort for the memory demand and the computing time, which is mainly caused by the high number of unknowns of the resulting system of equations in 3D, a high-performance computing framework for the application of the developed algorithms on high-performance computers is proposed to be analysed. The initial separation of sub-domains governed by their fundamentally different material behaviors leads to the separation and decomposition of elastic and inelastic subproblems. This enables a drastic reduction in global degrees of freedom (d.o.f.s) and, consequently, results in a significant decrease of the solution time. Furthermore, the author will use an initial and updated decomposed damage zone during the nonlinear (damage) simulation. This strategy should reduce the high memory demand required for storing all necessary history data, which can be extensive for large-scale FE models in 3D. The most time-consuming task of the computation procedure is the numerical solution of the underlying equation system, which also depends on the level of detail used for the discretized mechanical task. In recent years, the distributed computing based on the message-passing interface standard (MPI) has been proven valuable, enabling the distributed computation of linear equation systems, utilizing as many computational nodes available in a high-performance computing framework [4]. Consequently, a memory-advantageous iterative MPI-solver strategy based on the conjugate gradient method (CG) may be chosen and accelerated by an efficient preconditioning technique. In general, the parallelization techniques are based on standard overlapping or non-overlapping domain decomposition methods for FE problems. They can be improved by considering an elastic–inelastic domain split and thereby, enabling the decomposition of a reduced nonlinear domain.

Due to the fact that the solution of the linearized global equation system is the most time-consuming task in linear as well as nonlinear simulations (with the repeated solution of the linearized step), it is important to select an optimal combination of the solver, the preconditioning and the parallelization techniques as well as considering the architectural features of the hardware applied. However, direct parallel solvers [1] have the disadvantage of a high-memory demand induced by the direct factorization of the assembled matrices for each sub-domain. Therefore, the classical use of the Schur complement method (where the Schur complement matrix is explicitly extracted for each sub-domain) requires extensive computing time and memory demand. Due to the dense matrix structure of the Schur complement system it is difficult to store, to factorize and to solve the assembled Schur complement system directly. This issue has an increasing influence when the number of degrees of freedom is increasing. On the other hand, for iterative solution methods, the used preconditioning technique can be critical either with regards to computing time or to extensive memory demand (depending on the type of discretized problem). In this paper, firstly, a parallelized version of the preconditioned conjugate gradient method (PPCG) based on domain decomposition is used without explicitly building the Schur complement system. The iterative computation of the resulting equation system for the nonlinear problem is also executed by using the preconditioned conjugate gradient method (CG, [8,2]).

Finally, in this paper a parallelized HPC computing framework is applied for hybrid meshed and partitioned multiphase specimens, especially for the numerical evaluation of the qualitative initiation of damage effects in multiphase materials. Other approaches than the conventional way of modeling material nonlinearities [16], like the consideration of material discontinuities by using the extended finite element method (XFEM) or the classical material point based nonlinear simulation techniques such as the Newton–Raphson (NR), modified NR or arc-length methods often lead to numerical instabilities and convergence problems during the establishment of the nonlinear post-peak paths. Due to this, the saw-tooth softening approach introduced by Rots et al. [11] provides an alternative approach to model material nonlinearities in a sequential way due to the repeated computation of the stepwise modified linearized problem. By this, the realistic representation of softening branches for quasi-brittle materials can be reproduced. In this paper, a scalable version of the sequential linear analysis (SLA) will be implemented applied for the hybrid-meshed heterogeneous specimens for the representation of induced damage effects in a nonlinear simulation model. By this, the developed solver strategy will be also adapted for hybrid high-performance computing frameworks taking into account different parallel hardware architecture.

2. Finite element method and domain decomposition

2.1. Approximation of the Navier differential equation

Following the standard displacement based finite element methods, a linear system of equations is given with

$$Ku = f \tag{1}$$

where $K \in R^{n\times n}$ is the stiffness matrix,u $\in R^n$ the displacement vector and $f \in R^n$ the nodal load vector. If K is a regular, symmetric and positive definite matrix, the above equation can numerically be solved using direct or iterative solver techniques which are available in sequential and parallel algorithms. An alternative parallelization technique of such system results in the decomposition of the underlying finite element discretization by applying substructuring methods also known as domain decomposition methods for which an overview is given in [14,9,5]. The following section describes the Schur complement method which will be the base for the distributed computing model.

2.2. Schur complement method

The Schur complement operator [13] is basically a static condensation of the interior nodal d.o.f.s. to the boundary related d.o.f.s if a domain is decomposed in a fixed number of subdomains each with a corresponding Schur complement matrix. The assembly of such Schur complements considering all subdomains results in a reduced, reordered and dense Schur complement system of equations. By this, Eq. (1) can be divided in the following components, representing two different adjacent subdomains, which are denoted by $^{(1)}$ and by $^{(2)}$ and connected by a common boundary with assembled stiffness parts (denoted by $\tilde{}$)

$$\begin{pmatrix} K_{ii}^{(1)} & 0 & K_{ib}^{(1)} \\ 0 & K_{ii}^{(2)} & K_{ib}^{(2)} \\ K_{ib}^{(1)^T} & K_{ib}^{(2)^T} & \tilde{K}_{bb} \end{pmatrix} \begin{pmatrix} u_i^{(1)} \\ u_i^{(2)} \\ u_b \end{pmatrix} = \begin{pmatrix} f_i^{(1)} \\ f_i^{(2)} \\ \tilde{f}_b \end{pmatrix} \tag{2}$$