8th. World Congress on Computational Mechanics (WCCM8)
5th. European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS 2008)
June 30 – July 5, 2008
Venice, Italy

MULTI-CONSTRAINT MESH PARTITIONING AND HYBRID SOLUTION STRATEGIES FOR 3D SIMULATION OF HETEROGENEOUS MICROSTRUCTURES

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Keywords: *Heterogenous Materials, Microstructure, Mesh Partitioning, Domain Decomposition (DD).*

ABSTRACT

The numerical simulation of microstructure models in 3D require significant resources of memory as well as parallel computational power. Additionally the material heterogeneity induced by different material phases demand adequate computational methods for the discretization and solution process related to the resulting and highly nonlinear problem.

The proposed approach suggests to separate discretization/solution strategies for the decomposed model and to combine them efficiently into a hybrid solver package in order to enable finally the FE based damage analysis of such heterogenous materials. One important aspect should be to decompose the multi-phase agglomerate related to the applied solution technique for considering different damage effects, i.e. discrete interface cracking between grains and matrix material as well as non-local damaging in specific domains of matrix-only material.

An algorithm for multi-constraint mesh partitioning of a quasi microstructure of concrete will be presented, considering the different materials of a 4 phase model (quartz grains, matrix, interfaces and pores/imperfections, fig. 1), leading to an efficient decomposition as preparation for a hybrid solution technique. For the partitioning the data structure of an adaptive mesh has to be transferred in memory-efficient sparse graphs which could be weighted with several constraints, e.g. characterizing different material phases. Based on the decomposed model a Schur complement based Domain Decomposition for the solution process will be applied. Therewith it should be possible

to solve the partial problem in local region of nonlinearity (interface solutions) and couple them with iterative methods applied on regions of non-inelastic material.

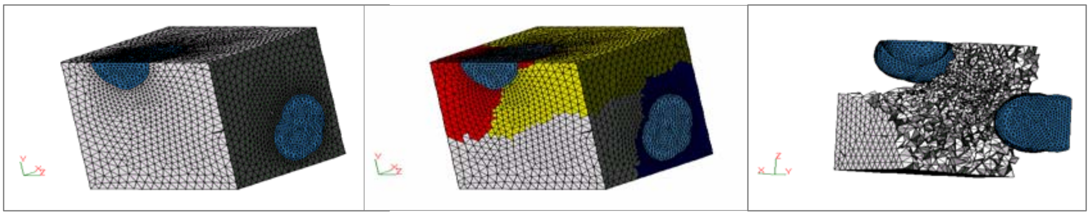

Fig. 1: Artificial heterogenous specimen with 2 inclusions (left) and the interface oriented decomposition of the adaptive mesh in 4 domains: Both aggregates as separate sub-structures and the second generated matrix-only domain (right).

Due to the heterogeneity of microstructures the resulting assembled and mostly fully occupied Schur matrix grows fast with higher numbers of generated domains by increasing the boundary problem which is one important disadvantage related to the global solving time. Thereby additional methods for the parallel solution process are required to avoid solving the global Schur equation system directly. Iterative substructuring methods like the Dirichlet-Neumann (D-N) and Neumann-Neumann (N-N) methods provide the advantage of Schur complement-free formulation, solving iteratively the D-N or N-N problem based on non-overlapping partitionings. Adopting these methods in a modified way should help reaching better results (i.e. memory demand, convergence rate) as this is the case by using classical Schur complement based DD procedures.

Futhermore the model can be adapted for the FE discretization and mechanical damage analysis of µCT based image data of real concrete samplings which should be the main task of future research activities.

ACKNOWLEDGEMENT

This research is supported by the German Research Foundation (DFG), which is gratefully acknowledged by the authors.

REFERENCES

[1] M. Formaggia, M. Sala, F. Saleri. (2005): *Domain decomposition techniques*, in: A. Bruaset, A. Tveito (Eds.), Numerical Solution of Partial Differential Equations on Parallel Computers, Lecture Notes in Computational Science and Engineering, vol. 51, Springer-Verlag, 2005, pp. 165–208.

[2] DDM - DOMAIN DECOMPOSITION: *Official page* (http://www.ddm.org). Contains information about annual int. Domain Decomposition meetings, links to proceedings, literature related to Domain Decomposition.