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# HPC in Computational Micromechanics of Composite Materials

(Poster Summary)

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## I. Introduction

By *micromechanics* we understand analysis of the macroscale response of materials through investigation of processes in their microstructure. Here by the macroscale, we mean the scale of applications, where we solve engineering problems involving materials. Examples could be analysis of aircraft constructions with different composite materials and analysis of rock behaviour and concrete properties in geo- and civil engineering applications. Analysis of bio-materials with many medicine applications is also rapidly developing. Different applications are distinguished by different characteristic size. At macroscale the materials mostly look as homogeneous or they are idealized as homogeneous or piecewise homogeneous. A substantial heterogeneity is hidden and appears only after more detailed zooming view into the material. This hidden heterogeneity can be called microstructure. In metals it is created by crystals and grains, in composite materials by matrix and inclusions, in concrete by gravel and mortar or iron reinforcement, in rock by mineral composition and possible grouting, etc. When the ratio between the characteristic dimensions on macro and microstructure subjects is sufficiently large, then we say that the scales are well separated. In this case, it is not possible to perform the macroscale analysis going into the microstructure details, but it is possible to analyse the macroscopic problems with the use of effective (homogenized) material properties, which are obtained by testing smaller samples of materials. In computational micromechanics, the testing of such samples means solution of boundary value problems on test domains involving the microstructure with loading provided by suitable boundary conditions.

In this work, we focus on X-ray CT image based micromechanics of geomaterials and concrete with the use of continuum mechanics and *finite element* (FE) computations of the microscale strains and stresses, see [2]. This means that basic information about the microstructure is provided by the analysis (segmentation) of 3D images of real samples. This information should be complemented by information on local material properties, i.e. material properties of the individual material constituents.

There is a strong need for high performance computing (HPC) at several levels of computational micromechanics, namely at:

- analysis of CT scans,
- high resolution finite element solution of boundary value problems,
- solution of inverse problems for determination or calibration of local material properties.

This contribution deals with the second point, i.e. solution of high resolution FE systems with tens or hundreds million *degrees of freedom* (DOF). We report about the performance of in-house solvers exploiting the *Schwarz domain decomposition method* with aggregation, c.f. [3], and outline possible future development in the area of *ultrascale computing*, which is necessary for building efficient solution methods for *inverse material identification problems*, see [4] and work in progress.

## II. High resolution FE systems

In the analysis of heterogeneous materials with microstructure *(composites)* (see [2]), our test sample domain $\Omega$ is a cube with a relatively complicated microstructure. Its FE mesh is constructed from data obtained from industrial CT scanning, performed at the CT-lab of the Institute of Geonics. Two types of composites are considered in this work: A *coal-resin* geocomposites and *reinforced concrete* composites. See Tab. 1 for the main characteristics of the resulting FE problems *(benchmarks)*.

| Benchmark | Discretization | Size in DOF | Data size |
|---|---|---|---|
| GEOC-2l | $257 \times 257 \times 1025$ | 203 100 675 | 33.5 GB |
| FIBER-3 | $401 \times 401 \times 401$ | 193 443 603 | 32.2 GB |

*Table 1: Benchmark problems: Name, discretization, size of the resulting linear system and storage requirements.*

The elastic response of a representative volume $\Omega$ is characterized by homogenized elasticity $C$ or compliance $S$ tensors ($S = C^{-1}$). The elasticity and compliance tensors are basically determined from the relations

$$C\langle\varepsilon\rangle = C\varepsilon_0 = \langle\sigma\rangle \quad \text{and} \quad S\langle\sigma\rangle = S\sigma_0 = \langle\varepsilon\rangle, \qquad (1)$$

respectively. Here $\langle\sigma\rangle$ and $\langle\varepsilon\rangle$ are volume averaged stresses and strains computed from the solution of elasticity problem

$$-\operatorname{div}(\sigma) = 0, \quad \sigma = C_m\varepsilon, \quad \varepsilon = (\nabla u + (\nabla u)^T)/2 \ \text{ in } \Omega, \qquad (2)$$

with boundary conditions

$$u(x) = \varepsilon_0 \cdot x \ \text{ on } \partial\Omega \quad \text{and} \quad \sigma \cdot n = \sigma_0 \cdot n \ \text{ on } \partial\Omega, \qquad (3)$$

respectively. Above, $\sigma$ and $\varepsilon$ denote stress and strain in the microstructure, $C_m$ is the variable local elasticity tensor, $u$ and $n$ denote the displacement and the unit normal, respectively. The use of pure Dirichlet and pure Neumann boundary conditions allows us to get a upper and lower bounds for the upscaled elasticity tensor, see e.g. [4].

## III. GEM solvers

*GEM* is an in-house FE software described in detail in [1], which makes use of linear tetrahedral finite elements for discretization. Arising systems of linear equations are processed by solvers based on the *preconditioned conjugate gradient* (PCG) method, with *stabilization* in the singular case [3]. PCG uses *overlapping domain decomposition preconditioners*. To solve the benchmarks, we employ two types of GEM solvers:

**GEM-DD** solver uses *one-level additive Schwarz* domain decomposition preconditioner with subproblems replaced by displacement decomposition incomplete factorization, see ref. in [3]. The resulting preconditioner is symmetric positive definite even for the singular case.

**GEM-DD+CG** solver implements *two-level Schwarz* domain decomposition preconditioning, arising from the GEM-DD above by additive involvement of a *coarse problem correction*. The coarse problem is created by a regular aggressive aggregation with 3 DoF' per aggregation. In the singular case, the coarse problem is also singular with a smaller null space containing only the rigid shifts. The coarse problem is solved only approximately by inner (not stabilized) CG method with a lower solution accuracy – relative residual accuracy $\varepsilon_0 \leq 0.01$.

## IV. Computing resources

The computations were performed on two parallel platforms:

**Enna** 64-core NUMA *multiprocessor*, Institute of Geonics AS CR: eight octa-core Intel Xeon E7-8837 / 2.66 GHz processors; 512 GB of DDR2 RAM; CentOS 6.3, Intel Cluster Studio XE 2013.

**Anselm** *multicomputer* (cluster, 209 compute nodes), IT4Innovations National Supercomputing Center: two octa-core Intel E5-2665 / 2.4 GHz processors per node; 64 GB RAM per node; Infiniband QDR interconnection, fully non-blocking, fat-tree; Bullx Linux Server 6.3 (Red Hat clone), Intel Parallel Studio 13.1.

## V. Computational experiments

Table 2 shows the timings of the GEM-DD+CG solver (with coarse grid problem applied) obtained for the **coal-resin geocomposite** benchmark GEOC-2l both on Enna and Anselm, and demonstrates the impact of the coarse grid size on the time of the solution. The *stopping criterion* $\|r\|/\|b\| \leq \varepsilon$, based on the relative residual accuracy, was $10^{-5}$. On Enna, the best results (2483.6 s) were observed with aggregation $9 \times 9 \times 9$.

| # Sd | Enna | | | | | | Anselm | |
|---|---|---|---|---|---|---|---|---|
| | DD + CG | | DD + CG | | DD + CG | | DD + CG | |
| | $9 \times 9 \times 9$ | | $9 \times 9 \times 18$ | | $9 \times 9 \times 27$ | | $9 \times 9 \times 27$ | |
| | # It | $T_{iter}$ | # It | $T_{iter}$ | # It | $T_{iter}$ | # It | $T_{iter}$ |
| 4 | 751 | 13719.0 | 858 | 15757.6 | 997 | 18518.4 | 997 | 12671.4 |
| 8 | 690 | 6237.7 | 800 | 6960.8 | 917 | 8062.9 | 917 | 5803.9 |
| 16 | 585 | 2717.4 | 674 | 4010.6 | 777 | 4815.6 | 777 | 2576.6 |
| 32 | 585 | **2483.6** | 622 | 2923.8 | 708 | 3452.5 | 708 | 1157.5 |
| 64 | | | | | 627 | 3637.0 | 627 | 558.8 |
| 128 | | | | | | | 652 | 358.5 |
| 256 | | | | | | | 631 | **299.6** |
| 512 | | | | | | | 649 | 333.5 |

*Table 2: Timings of the GEOC-2l benchmark with pure Neumann boundary conditions and achieved by the GEM-DD+CG solver on the multiprocessor Enna and multicomputer Anselm: Iteration counts (# It) and wall-clock time (in seconds) for the solution time ($T_{iter}$) are provided now for different sizes of CG problem involved in computations and for various numbers of subdomains (# Sd).*

The experiments confirm the advantage of multicomputers (systems with distributed memory) for greater number of subdomains, when the multiprocessors in general suffer from the memory-processor bandwidth contention. Thus, while on Enna the scalability fades out at about 32 cores, the turning point on Anselm is around 256 processing elements, when the small size of subdomains deteriorates the ratio between computation and communication. In absolute figures, we were able to solve the benchmark 8 times faster on Anselm than on Enna. A part of Anselm's advantage is to be credited to its newer Intel Sandy Bridge CPU architecture, which outperforms Enna's Westmere CPU in our applications by 20 - 40 % (separate test).

A bit surprising decrease of the number of iterations with increasing number of subdomains (processors) as reported in the above Tables, can be explained by the fact that smaller subdomain problems are solved more accurately in our implementation.

Anselm/GEOC-2l best time in Table 2 (299.6 s with 256 processing elements and aggregation $9 \times 9 \times 27$) was surpassed by another experiment (not shown in the table): aggregation $15 \times 15 \times 31$, 910 iterations, 512 subdomains (32 compute nodes employed), **249.8 s**.

The experiments carried out on the **fiber-reinforced concrete** FIBER-3 benchmark delivered similar results. So far, just Enna has been used for computations, confirming limited scalability on its multi-processor architecture. We observed great importance of the coarse grid and its proper dimensioning for efficient solution (computing times of GEM-DD are multiples of the computing times of GEM-DD+CG).

## VI. Conclusions and future work

Micromechanics leads to large-scale problems, as illustrated by the presented benchmarks. The computational requirements can be further substantially increased in the case of an *inverse analysis for identification local material properties* (see e.g. [4]).

At the IT4Innovations National Supercomputing Center, there is a new massively parallel computer available, called Salomon. This multi-computer (cluster) has 1008 compute nodes and we plan to employ it in future experiments.

The approach described so far employs classical domain decomposition philosophy. Both facts, computational demands and availability of massively parallel computers, motivate further research in algorithms, which are efficient from the point of view of arithmetic operations and (even more important) from the point of view of communication.

In the future, we plan to test the effect of *communication avoiding* (CA) algorithms. For example, using the same ingredients as in our domain decomposition solvers, we can employ CA conjugate gradients and a deflation type implementation of the aggregation based coarse space.

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