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Multigrid solution of the 3D stress field in strongly heterogeneous materials

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ABSTRACT

Technology allows the production of advanced (heterogeneous) materials controlling properties on an increasingly local scale, e.g. layered, graded, granular and fiber-reinforced. In this paper the efficiency of the Multigrid method for 3D stress calculation involving such materials is investigated. Results are validated using model problems and the full potential is demonstrated for two representative problems. The developed algorithm facilitates solution of 3D problems with high accuracy and dense grids on standard computers. It has excellent prospects for use in performance prediction, analysis and numerical (local) design optimization in tribology and contact mechanics.

1. Introduction

Numerical simulations nowadays play a significant role for the design and optimization of structures and machine elements. Advanced technology of material production allows control of the microstructure of materials at an increasingly detailed level, to create components with a tailored distribution of (local) properties, e.g. coated, graded, granular, porous, fiber reinforced and composite materials. The analysis and the prediction of the behavior of machine elements or structural elements made up of heterogeneous materials under different operating conditions (mechanical and thermal) is a topic of study in many areas in engineering, e.g. in material science, biomechanics, structural mechanics, contact mechanics and tribology.

In many studies the development of computer simulation methods is described. For example, Roux [1] and De Roeck et al. [2] developed methods in which the (many) subdomains with different properties are considered separately, and linked via interface conditions which ensure the continuity of the displacements. In [3] this continuity is imposed through Lagrange multipliers [3]. Molinari et al. [4,5] and Sadeghi et al. [6–8] developed approaches to determine stress and strain fields in polycrystalline materials. There are many other examples in the engineering literature.

These studies have demonstrated that the investigation of local phenomena in heterogeneous materials, e.g. in a small volume composed of grains, is feasible, with today's computer methods and fast computers. However, the geometrical complexity of the local structure and the need for an accurate solution require the use of a very fine discretization (element mesh). Especially for three-dimensional problems this leads to large systems of equations with (many) millions of unknowns which, using standard methods of e.g. (band)matrix inversion, require large computing times to solve. The use of supercomputers and extensive parallelization alleviates this problem but, to bring these methods to application as a computational tool for design and optimization in an engineering environment, much more efficient and faster solution methods are needed so that realistic problems can be solved on small scale computers.

Multigrid techniques were introduced in the early seventies by Brandt [9] for scalar elliptic equations and have since been applied and further developed to many fields in science and engineering. The techniques have the prospect of solving a problem in a computing time proportional to the number of degrees of freedom, which makes them well suited for 3D problems. An introduction to Multigrid is given in [10]. Advanced reading can be found in [11–13]. For applications in structural mechanics see e.g. [14].

The concept is to use (simple) iterative solvers and to obtain very fast convergence and high efficiency by the design of an efficient way to approximate and solve the slow to converge error components using a coarser scale. For elliptic problems these are generally smooth error components for which coarser grids are used, hence the name Multigrid. The coarser scales may also be generated from the original system of equations in what is called Algebraic Multigrid (AMG) as opposed to geometric Multigrid. AMG algorithms are less problem specific and can be applied to general problems only specified in matrix vector form. However, they are also computationally more expensive.

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Nomenclature

$E_{x,y,z}$	Young's modulus
P_0	maximum Hertzian pressure
a_0	Hertzian contact radius
i,j,k	index in x–y–z direction
u,v,w	displacements in x–y–z direction
$\lambda_{x,y,z},\mu_{x,y,z}$	Lamé coefficients
L_x,L_y,L_z	volume dimensions in x–y–z direction
h	grid spacing
Ω	computational domain
$\partial\Omega$	boundary of the domain

The objective of the present study is to develop a fast efficient solver to deal with 3D strongly heterogeneous elastic problems based on *geometric* Multigrid techniques for use in heterogeneous material analysis, optimization and design, and computational diagnostics. In previous work, Boffy et al. [15] demonstrated the efficiency for computing the stress field in materials subjected to an imposed contact pressure for coated and graded materials with low property ratios. However, with increasing property ratios the efficiency of standard geometric Multigrid deteriorates. In this paper it is explained how efficiency can be retained when the property variations are large.

First, the Lamé equations for 3D solids with arbitrary graded elasticity are described and the relevant details of the Multigrid algorithm are explained. To demonstrate the accuracy first results are presented for characteristic problems taken from the literature. Next, to demonstrate the real potential of the developed algorithm results are presented involving heterogeneous media with small and large mechanical property ratios. Two cases are considered: an application from contact-mechanics of a granular material with interstitial matter subjected to an external pressure, and the analysis of a (piece of) fiber reinforced material in which the fiber orientation is varied. The results demonstrate the efficiency of the developed algorithm allowing detailed simulations in 3D to be carried out on a small scale single processor computer. The developed algorithm has great potential to contribute to the analysis, design and optimization of new materials.

2. Theoretical model

The 3D heterogeneous linear elastic problem can be described as the solution of the unknown displacements u, v and w in a 3-D domain Ω from the Navier–Cauchy equations:

$$(\lambda u_{j,j})_{,i}+(\mu u_{i,j})_{,j}+(\mu u_{j,i})_{,j}=0,\quad i,j=1,2,3 \tag{1}$$

where λ and μ are the Lamé coefficients, which are assumed to vary as a function of space

$$\lambda(x,y,z)=\frac{E(x,y,z)\nu(x,y,z)}{(1+\nu(x,y,z))(1-2\nu(x,y,z))} \tag{2}$$

$$\mu(x,y,z)=\frac{E(x,y,z)}{2(1+\nu(x,y,z))} \tag{3}$$

Typically, Ω will be taken as a 3-D rectangular domain, representative of a section of a heterogeneous material.

Assuming a Cartesian coordinate system, for the case of $i=1$, Eq. (1) can be written as

$$\frac{\partial}{\partial x}\left[(\lambda+\mu)\left(\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}+\frac{\partial w}{\partial z}\right)\right]+\frac{\partial}{\partial x}\left(\mu\frac{\partial u}{\partial x}\right)+\frac{\partial}{\partial y}\left(\mu\frac{\partial u}{\partial y}\right)+\frac{\partial}{\partial z}\left(\mu\frac{\partial u}{\partial z}\right)=0 \tag{4}$$

On the boundary $\partial\Omega$ of the domain, both Neumann and Dirichlet boundary conditions (BC) can be considered, depending on the specific application, i.e. imposed stress/friction at a surface or free displacement, or imposed displacement.

3. Multigrid numerical solution

The system of equations was discretized on a uniform grid with mesh size h in each spatial direction. This choice was motivated by simplicity and memory efficiency. A finite difference discretization was used of second order accuracy, with the equations and each of the unknowns defined at the grid points (see Appendix). This choice is adequate for most practical materials with Poisson ratio's $0.25\le\nu\le0.45$. For nearly incompressible materials ($\nu\approx0.5$) the discretization should be a staggered configuration to avoid spurious oscillations, see [11,16]. Let the system of equations be written as

$$L^h\mathbf{u}^h=0\quad\text{on }\Omega^h \tag{5}$$

where L^h is a matrix and $\mathbf{u}^h$ is a vector containing the displacements to be solved in the grid points. The solution of $\mathbf{u}^h$ using direct methods requires an amount of work $O(b^2N)$ where b is the bandwidth of the matrix and N the total number of unknown. Usually $b=O(N^{(d-1)/d})$ which leads to excessive computing times for 3D problems with dense grids. Iterative methods such as Gauss–Seidel relaxation are also computationally expensive, because of slow convergence. Components which are near the eigenspace of the matrix (operator) converge at a rate strongly decreasing with the mesh size. For elliptic problems these are the smooth error components. High frequency error components on the other hand are very efficiently reduced. Geometric Multigrid techniques exploit this behavior by introducing a sequence of coarser grids to resolve the slow to converge smooth errors at coarser grid where this can be done more efficiently and use the result to correct the fine grid solution, see Fig. 1. This coarse grid correction concept is applied recursively yielding a coarse grid correction cycle using multiple grids which has grid independent fast convergence. Multigrid algorithms are not black-box solvers. Various aspects need to be considered carefully to achieve good efficiency. These aspects of (geometric) Multigrid algorithm development for the 3D elasticity problem are discussed below.

3.1. Relaxation

The iterative process used should reduce all error components that cannot be seen on the coarse grid with $H=2h$ where H is the

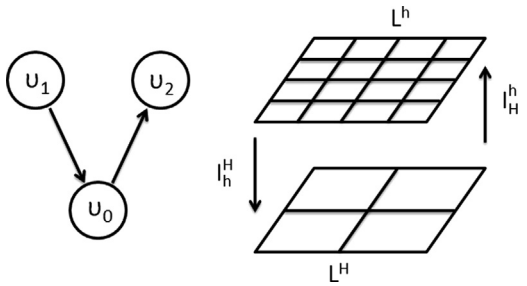

Fig. 1. Generic representation of a Multigrid V-cycle 2 levels with interpolation I_H^h and restriction I_h^H operators. ν_1 and ν_2 are respectively the numbers of relaxations used to smooth the error before coarsening and remove errors introduced by the interpolation of the correction. $\nu_0=\nu_1+\nu_2$. L_H and L_h represent the operators used to solve the equations on the coarse and fine grid respectively.