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Preconditioned conjugate gradient method enhanced by deflation of rigid body modes applied to composite materials

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Abstract: The introduction of computed x-ray tomography allows for the construction of high quality, material-per-element based 3D meshes in the field of structural mechanics. The use of these meshes enables a shift from meso to micro scale analysis of composite materials like cement concrete, rocks and asphalt concrete. Unfortunately, because of the extremely long execution time, memory and storage space demands, the majority of commercially available finite element packages are not capable of handling efficiently the most computationally demanding operation of the finite element solution process, that is, the inversion of the structural stiffness matrix.

The linearized virtual work equation gives a symmetric positive definite (SPD) stiffness matrix. Because of these properties of the stiffness matrix we use preconditioned CG (PCG) as the initial solver. The PCG solver has an excellent performance on SPD matrices, is cheap in terms of work and is highly parallelizable. The error of PCG is bounded by the condition number of the stiffness matrix. Increasing the stiffness of the materials results in a higher condition number, yielding worse performance. However, the number of aggregates seems to have no influence on the value of the condition number.

Our numerical experiments show that the performance of CG with a diagonal scaling preconditioner is poor. Increasing the stiffness as well as the number of aggregates results in a deterioration of the convergence rates of PCG. The results also show plateaus in the convergence behavior which indicates the existence of small eigenvalues related to slow converging components. Analysis of the spectrum of the preconditioned stiffness matrix shows that the smallest eigenvalues correspond to the domains containing aggregates. Moreover, the number of small eigenvalues is equal to the number of rigid body modes of the aggregates.

The performance of PCG can be improved by removing the smallest eigenvalues from the spectrum of the stiffness matrix. We use deflation based preconditioners to filter out those values. All vectors in the deflation subspace are projected out of the residual of the iterative process. We use the rigid body modes for the disjunct aggregates as the deflation subspace. The removal of the rigid body modes results in a mechanical and mathematical well defined problem that only depends on the material properties of the bitumen. The convergence behavior of DPCG is identical to the convergence behavior of a homogeneous material benchmark case. Adding more and stiffer aggregates has no effect on the performance of DPCG. We have constructed an iterative solver which has aggregate independent convergence behavior. Furthermore, this is the first application of deflation based preconditioning applied to coupled systems of partial differential equations.

Keywords: *Rigid body modes, Preconditioned conjugate gradient method.*

Abstract only