SOLVING MULTISCALE PROBLEMS WITH MILLION-WAY CONCURRENCY

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ABSTRACT

Robust parallel algorithms and software will be discussed with applications in materials science, i.e., for the design of tougher and lighter materials. A focus is on highly parallel methods to enable detailed micro-macro simulations of modern, heterogeneous materials on today's supercomputers and on those of the upcoming exascale era. Here, the well-known FE^2 computational micro-macro scale bridging approach is combined with highly parallel scalable nonlinear and linear iterative solvers [1, 2, 3, 4, 5]

In this approach, a microscopic boundary value problem based on a representative volume element (RVE) is solved at each macroscopic Gauss integration point. Then, nonlinear nonoverlappicng domain decomposition methods of the FETI-DP type, combined with linear multigrid methods, are applied to solve nonlinear hyperelasticity or plasticity problems on the RVEs. In nonlinear domain decomposition methods the nonlinear problem is decomposed into parallel nonlinear problems before Newton linearization increasing locality and reducing communication. Parallel scalability to millions of MPI ranks is achieved for heterogeneous multiscale problems with billions of unknowns.

We use new nonlinear domain decomposition solvers in our approach [5]. For a few decades already, Newton-Krylov algorithms with suitable preconditioners such as domain decomposition (DD) or multigrid (MG) methods (Newton-Krylov-DD or Newton-Krylov-MG) have been the workhorse for the parallel solution of nonlinear implicit problems. In these methods the nonlinear problem is first linearized and then decomposed. By changing the order of these operations, new algorithms with increased locality and reduced communication are obtained. Moreover, reductions on energy to solution can be observed.

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