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HIGH ORDER EDGE ELEMENTS AND DOMAIN DECOMPOSITION PRECONDITIONING FOR THE TIME-HARMONIC MAXWELL'S EQUATIONS

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Edge elements are finite elements particularly suited for the approximation of the electric field, and high order elements provide, at a fixed number of unknowns, a more accurate solution. The high order generators presented in [1] have a rather simple expression since they are defined only in terms of barycentric coordinates, and a convenient set of degrees of freedom can be chosen to facilitate their implementation in the finite elements framework (see [2] for practical details).

However, the matrices of the linear systems resulting from this high order discretization are ill conditioned, so that preconditioning becomes necessary when using iterative solvers. Indeed, direct solvers are more robust, but for the considered large scale simulations they can't be used since they require a high memory cost. As preconditioners we choose domain decomposition preconditioners, which are naturally suited for parallel computing and make it possible to deal with smaller subproblems. We present numerical results for the simulation of Maxwell's equations in high frequency regime and for dissipative and heterogeneous media (the tests were performed on the Curie supercomputer of GENCI-CEA).

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SCHWARZ PRECONDITIONER WITH HARMONICALLY ENRICHED MULTISCALE COARSE SPACE

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In this presentation, we will consider the second order elliptic boundary value problem in 2D and 3D with highly varying and heterogeneous coefficients, and present variants of the harmonically enriched multiscale coarse space for the additive Schwarz preconditioner for the problem. The preconditioner is based on the abstract Schwarz framework. For the coarse space we propose to use the standard multiscale finite element function or its variants, and show how to enrich the coarse space in order to construc t preconditioners that are robust with respect to any variations and discontinuities in the coefficients. The harmonic enrichment is based on solving certain, simple, but carefully chosen, lower dimensional generalized eigenvalue problems on the interfaces between subdomains. Convergence analysis and the numerical results supporting the analysis will be presented.

BLOCK ITERATIVE METHODS AND RECYCLING FOR IMPROVED SCALABILITY OF LINEAR SOLVERS

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On the one hand, block iterative methods may be useful when solving systems with multiple right-hand sides, for example when dealing with time-harmonic Maxwell's equations. They indeed offer higher arithmetic intensity, and typically decrease the number of iterations of Krylov solvers. On the other hand, recycling also provides a way to decrease the time to solution of successive linear solves, when all right-hand sides are not available at the same time. I will present some results using both approaches, as well as their implementation inside the open-source framework HPDDM (https://github.com/hpddm/hpddm). Combined with efficient preconditioners based on domain decomposition or algebraic multigrid methods, linear systems with tens of millions of unknowns are solved to assess the efficiency of the framework.

TIME PARALLELIZATION OF SCHWARZ WAVEFORM RELAXATION METHODS

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Schwarz waveform relaxation (WR) methods, as well as the related Neumann-Neumann WR method, are domain decomposition methods for solving time-dependent PDEs in parallel. By dividing the computational domain into many subdomains, one can solve the time-dependent PDE in each subdomain separately, and in parallel, over a given time window. The subdomains then exchange interface data, and we iterate until a consistent global solution is obtained. Unlike classical parallelization approaches where the same time step is used for the whole domain and domain decomposition is only applied to the spatial problem, WR methods permits the use of different spatial and time discretizations for different subdomains. Moreover, WR methods have been shown to converge superlinearly to the single domain solution over finite time windows, although convergence deteriorates as the time window size increases.

In this talk, we first show how WR methods can be parallelized naturally in time by running several iterations simultaneously. This allows an additional direction of parallelization, after saturation in the spatial direction. Next, we observe that because of the superlinear convergence of WR methods, the error in fact decreases much faster to zero at the beginning of the time window than at later times. Thus, with the help of a posteriori error estimates, it is possible to detect when the error has dropped below a given tolerance over some part of the time window. This allows us to stop iterating in the parts where the solution has converged and reduce the effective time window size, and hence the overall computational time. Finally, we show numerical examples to illustrate our approach.

OPTIMIZED SCHWARZ AND 2-LAGRANGE MULTIPLIER METHODS FOR MULTISCALE ELLIPTIC PDES

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Elliptic partial differential equations (PDE) describe the long-term evolution of a diffusion or heat problems. The medium through which the fluid is flowing is said to be heterogeneous if it consists of a mixture of several substances through which the fluid flows at varying rates. For example, a heterogeneous soil may consist of layers of sand (through which water flows quickly) and rock (through which water diffuses very slowly).

Domain decomposition is a method for solving elliptic PDEs in parallel in an efficient manner. The basic idea is to partition the overall domain Ω into many subdomains $\Omega = \cup_k \Omega_k$ and to solve the PDE iteratively on each subdomain in parallel. In optimized Schwarz methods (OSM) and 2-Lagrange multiplier methods (2LM), the boundary conditions on $\partial\Omega_k$ are of the Robin type. For a suitable choice of Robin parameter, one obtains a method that converges faster than a classical Schwarz iteration.

In order to obtain good parallel scaling, the Schwarz method must be combined with a “coarse grid correction”, which serves to accelerate the convergence of the low frequencies. However, when the PDE is heterogeneous, some “fast-moving modes” are indeed “low frequency” (e.g. it does not take very much energy for water to flow through sand). This means that the coarse space must contain some nontrivial fast-moving but low frequency modes.

One way to capture such modes in the coarse space is to find a few low-energy eigenvectors for the Dirichlet-to-Neumann map of each subdomain Ω_k. We show how one can use such a coarse space for OSM and 2LM and thus obtain arbitrarily fast convergence for heterogeneous problems.

THE HYBRID TOTAL FETI METHOD IN ESPRESO LIBRARY

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We present our hybrid variant of the Total FETI method, firstly proposed by A. Klawonn and O. Rheinbach [2]. The original algorithm combines the FETI [3] and FETI-DP [4] method to treat the coarse problem in a more optimal way. Briefly said, the hybrid FETI method connects several neighbouring subdomains into clusters (using the FETI-DP approach), so each cluster behaves like one subdomain, and therefore the global coarse problem depends on the number of clusters and not on the number of subdomains. We present a slightly different variant of the algorithm [5], in which the FETI method is used on both levels. It allows the method to bond two or more subdomains into clusters differently, e.g., per the whole common face between each two neighbouring subdomains on average.
The numerical results presented in the talk were obtained via in-house developed ESPRESO library [1]. This library is a highly efficient parallel solver containing several FETI method based algorithms including the HTFETI method able to solve problems over billions of unknowns. The solver is based on a highly efficient communication layer based on MPI, and it is able to run on massively parallel machines with thousands of compute nodes and hundreds of thousands of CPU cores. ESPRESO is also being developed to support modern many-core accelerators.

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PHYSICS-BASED BALANCING DOMAIN DECOMPOSITION BY CONSTRAINTS FOR HETEROGENEOUS PROBLEMS

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Solving a PDE with heterogeneous coefficient is challenging. On the one hand, the size of the associated linear systems can be very large as a fine mesh is often required to represent all of the different scales in the coefficient. On the other hand, the high contrast and rapid variation of the coefficient can greatly increase the condition number of the associated linear system, makes it difficult to solve by iterative solvers. Therefore, robust parallel preconditioners are needed for this type of problems. In this talk, we present a balancing domain decomposition by constraints (BDDC) method based on aggregation of elements with the same or "nearly" the same coefficient. Instead of imposing constraints on purely geometrical objects (faces, edges and vertices) of the partition interface, we use interface objects (subfaces, subedges and vertices) defined by the variation of the coefficients. When the coefficient is constant in each object, we can show both theoretically and numerically that the condition number does not depend on the contrast of the coefficient. In cases where the constant coefficient condition results in too many objects (a large coarse problem), we relax the condition and only require that the ratio of the minimal and maximal values of the coefficient in each object larger than a predefined threshold. The threshold can be chosen so that the condition number is reasonably small while the size of the coarse problem is not too large. We emphasize that the new method is easy to implement and does not require to solve any eigenvalue or auxiliary problems. Numerical experiments are provided to support our findings.

AN ADAPTIVE MULTIPRECONDITIONED CONJUGATE GRADIENT ALGORITHM AND ITS APPLICATION TO DOMAIN DECOMPOSITION

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I will show that for realistic simulations (with heterogeneous materials for instance) convergence of domain decomposition methods becomes very slow. Then I will explain how this can be fixed by injecting more information into the solver. In particular, robustness can be achieved by using multiple search directions within the conjugate gradient algorithm. Efficiency is also taken into account since our solvers are adaptive.

This work is a particular application of the adaptive multipreconditioned conjugate gradient algorithm [2, 1].

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