Towards Black-Box Direct Domain Decomposition Methods

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Large sparse linear systems arise in many STEM disciplines when a natural or manmade system under investigation can be described (modeled) either via differential equations (DE), e.g. electromagnetic radiation and scattering, or a graph representation of the interactions among its items/parts, e.g. the internet and social networks. In the former cases where DEs are involved, the goal of modeling is often to find the system's response under a known stimulus (system solution) or find its natural response (eignesolution) or even some characteristics of the system itself when the responses of known stimuli are measured (inverse problem). For those type of problems, factorizing the sparse matrix (e.g. LU or LDL^T or even Cholesky factorization), of the underlying linear system of equations is be the most reliable and often efficient avenue for solving the problem.

Several efficient algorithms for each of the above sparse matrix factorizations,(all with the same asymptotic complexity) have been implemented into highly optimized 'black-box' linear algebra libraries or software packages. Those mostly rely on the super-nodal or multi-frontal implementations of the appropriate factorization, and are coupled with advanced matrix reordering, scaling or pivoting schemes. Despite remarkable advances, direct solution is almost always the memory bottleneck of a simulation, with $O(N^2)$ worst-case asymptotically scale and offer only moderate parallel speed-ups. Although the scaling is a fundamental problem that likely can not be improved in numerically exact arithmetic, there is enough evidence to suggest that the memory and parallel speed-up bottlenecks can be remarkably improved.

Recently, our group has shown that specialized (to DE) direct solvers for general FEM electromagnetic, with the aid of direct domain decomposition methods (D^3M), can indeed outperform state-of-the-art 'black-box' direct solver libraries in terms of memory and parallel speed-up (J. Moshfegh and M. N. Vouvakis, Direct domain decomposition method (D3M) for finite element electromagnetic computations, 2016 IEEE (APSURSI)). These direct solvers though, require a certain ad-hoc geometric partitioning prior to discretizing or solving the problem, making them somewhat more cumbersome 'black-box' direct solver.

The broader scientific question that this paper aims to address is, can D^3M be a general 'back-box' direct solver, that is not only applicable to DE discretization schemes, but any non-singular linear system of equations, while maintaining or improving the memory and parallel efficiency demonstrated in early experiments? This paper will inch a step closer towards answering this question, by re-formulating D^3M for FEM problems that are not geometrical partitioned, thus allowing D^3M to control the best possible mesh partitioning. One on had, this removes the cumbersome partitioning step, that is now left to the user, but likely exposes the method to arbitrary perhaps larger separators that may degrade efficiency. The talk will present algorithms and numerical results that shed light into this question.