Direct Domain Decomposition Method (D³M) for Finite Element Electromagnetic Computations

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Abstract—An exact arithmetic, memory efficient direct solution method for finite element method (FEM) computations is outlined. Unlike conventional black-box or low-rank direct solvers that are opaque to the underlying physical problem, the proposed method leverages physical insights at every stage of the development through a new symmetric domain decomposition method (DDM) with one set of Lagrange multipliers. Comparisons with state-of-the-art exact direct solvers on electrically large problems suggest up to 10 times less memory and better run-time complexity while maintaining the same accuracy.

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I. INTRODUCTION

Modern computational electromagnetics FEM tools often rely on memory efficient iterative solvers such as Multigrid and DDM that may experience convergence difficulties near resonances or multi-scale problems, and lose efficiency at multiple excitation runs. Contrary, direct solvers such as MUMPS or PARDISO are reliable but scale unfavorably and are hard to parallelize. Thus, recent trends in direct solvers strive to reduce workload by leveraging low-rank approximations at the cost of accuracy and possibly reliability. Yet, these solvers are opaque to important underlying physics, leaving room for further improvements.

To achieve an efficient exact direct solver, one must start from scratch and attempt to leverage deep physical and numerical insights that may require re-formulating the BVP and FEM assembling, in addition to the symbolic and numeric factorization stages. This is critical not only to avoid internal resonances at all intermediate factorization separators, but also to produce numerically efficient matrix structures i.e. reduced size, block-wise sparse symmetric matrices.

This work achieves all these via a direct DDM (D³M) framework. A set of auxiliary variables is used to cast a decomposed BVP that, after an initial reduction/elimination step, leads to an auxiliary blocked matrix that is suitable for factorization. To attain maximal performance, this matrix is factored with a special blocked LDL⁺T method with restricted Bunch-Kaufman pivoting.

The accuracy and performance of the proposed D³M has been verified and tested in 3D scattering problems by perfect electric conductor (PEC) plates and dielectric spheres of progressively larger electrical sizes. The proposed D³M solver requires 3×−10× less memory than MUMPS mainly due to the choice of structured separators and the absence of delayed pivots attributed to the interior resonance free formulation. An initial serial implementation of D³M was up to two times slower than MUMPS for small problems but becomes competitive on problems larger than one million unknowns.

II. THEORY

Consider a computational domain Ω decomposed into N non-overlapping subdomain Ωi. For example, a decomposed problem with four domains is shown in Fig. 1. The decomposed BVP reads, find (E,λ) ∈ {V,λ} such that:

\[
\begin{align*}
\nabla \times \frac{1}{\varepsilon} \nabla \times E_i - k^2 e_i E_i &= -j k \eta J^{imp}, & \text{in } \Omega = \bigcup_{i=1}^{N} \Omega_i \\
\gamma_x (\nabla \times E_i) - j k \gamma_t (E_i) &= \gamma_x (\nabla \times E^{inc}_i) - j k \gamma_t (E^{inc}_i), & \text{on } \partial \Omega \\
R^{(i)}_{ij} [j - \alpha \eta] - R^{(N(i))}_{ij} [-j - \alpha \eta] &= 0, & \text{on } S, \forall i \& \{ij\} \\
R^{(i)}_{ij} e - R^{(N(i))}_{ij} e &= 0, & \text{on } S, \forall i \& \{ij\}
\end{align*}
\]

where \( e = \gamma_t (E|S) \), and \( j = \gamma_x (\nabla \times E|S) \). \( R^{(i)}_{ij} \) is the restriction operator from domain \( i \) to interface \( ij \), and \( N(i) \) denotes the neighbor of domain \( i \).

After transforming to \( \lambda = j \pm \epsilon \), casting the variational problem and expanding trial and testing function spaces gives

\[
\begin{bmatrix}
A & D \\
D^T & 0
\end{bmatrix}
\begin{bmatrix}
E \\
0
\end{bmatrix}
\rightarrow
f_{elim} E \\
\rightarrow
\begin{bmatrix}
N \end{bmatrix}
\begin{bmatrix}
A_i \\
D_i
\end{bmatrix}
^{-1}
\begin{bmatrix}
D_i \\
0
\end{bmatrix}
\lambda = g. \quad (1)
\]

where \( A \) is the diagonal blocked matrix of \( A_i, i = 1, 2, ..., N \) where \( A_i \) is the FEM-ABC matrix for domain \( i \) with loss or gain at the interfaces. \( D \) is a blocked matrix of sparse matrices \( D_i, i = 1, 2, ..., N_i \) which maps the primal space to LM space. \( N_i \) is the number of interfaces.

The reduced matrix \( K \) is symmetric block-wise sparse but indefinite. Hence LDL⁺T factorization with symmetric partial pivoting a.k.a Bunch-Kaufman LDL⁺T [6] can be used to save
memory and CPU time. Since $K$ is a block-wise sparse matrix, we have modified the Bunch-Kaufman LDL$^T$ factorization to its block restricted partial pivoted form. Each block in $K$ corresponds to a super-node of typical order $n > 300$. Therefore, D$^3$M consistently operates at the maximum performance region of Level 3 BLAS. The main steps of the proposed D$^3$M are:

1) Generate dense domain matrices $K^{(d)}_{D}$,
2) Assemble the block-wise sparse reduced matrix $K$,
3) Reorder the clique graph of $K$,
4) Symbolic factorize the reordered clique graph,
5) Factorize $K$ with restricted B-K pivoting block LDL$^T$ factorization (see algorithm 1),
6) Forward/Backward substitute the reduced system $K$ for auxiliary unknowns,
7) Recover primal unknowns.

The clique graph of blocked sparse matrix $K$ is reordered using METIS (same as MUMPS). Assuming that the clique graph has $l$ levels, the algorithm of block LDL$^T$ factorization is given in Algorithm 1. A multifrontal version of block LDL$^T$ can be used to further speed computations.

Algorithm 1 Block LDL$^T$ factorization

```plaintext
for $j = 1 \rightarrow l$ do
  Dense LDL$^T$ factorize $K_{jj}$
  for $\forall i | K_{ij} \neq 0$ do
    Dense Triangular solve $L_{ij}X_{ij}^T = K_{ij}^T$, for $X_{ij} = P_{ij}L_{ij}D_{ij}$
    Compute work variable $W_{ij} = X_{ij}D_{ii}^{-1}$
    for $\forall k | K_{ik} \neq 0$ do
      Dense update $K_{ik} \leftarrow A_{ik} - X_{ij}W_{ij}^T$
    end for
  end for
end for
```

III. Numerical Results

First, the scattering of progressively larger PEC plates (from $3\lambda \times 3\lambda$ up to $19\lambda \times 19\lambda$) are considered. Computational complexity of factorization time and memory for these problems using the proposed D$^3$M and MUMPS are shown in Fig. 2. It is noted that a 3M unknown problem is solved with only 10 GB of RAM at full double precision accuracy.

Next, the scattering of progressively larger dielectric spheres is considered. Computational complexity of factorization time and memory for these problems using the proposed D$^3$M and MUMPS are shown in Fig. 3. Again, the proposed method uses more than 2.25 times less memory and surprisingly better time complexity than MUMPS. The relative residual error $(\|A\bar{x} - f\|_{inf} / \|f\|_{inf})$ of all runs using the proposed D$^3$M is around $10^{-12} - 10^{-13}$ which was the same as MUMPS.

**References**

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