A parallel hybrid linear solver for EM simulations

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In ComPASS EM simulations, solving linear systems is often memory bottleneck:

\[ Ax = b, \]

where \( A \) is

- **sparse but large**
  - direct methods are robust, but require large memory.

- **ill-conditioned and highly-indefinite**
  - preconditioned iterative methods require less memory, but suffer from slow or no convergence.

**Hybrid method** has the potential of balancing robustness of direct methods with efficiency of preconditioned iterative methods.
**Schur complement method**: reorder $A$ into a $2 \times 2$ block system:

\[
\begin{pmatrix}
A_{11} & A_{12} \\
A_{21} & A_{22}
\end{pmatrix}
\begin{pmatrix}
x_1 \\
x_2
\end{pmatrix} =
\begin{pmatrix}
b_1 \\
b_2
\end{pmatrix}
\]

where

- $A_{11}$ is *interior domains*, $A_{22}$ is *separators*, and $A_{21}$ and $A_{12}$ are the *interfaces* between $A_{11}$ and $A_{22}$ such that

\[
\begin{pmatrix}
A_{11} & A_{12} \\
A_{21} & A_{22}
\end{pmatrix} =
\begin{pmatrix}
A_{11}^{(1)} & A_{12}^{(1)} & A_{11}^{(2)} & A_{12}^{(2)} \\
A_{21}^{(1)} & A_{22}^{(1)} & A_{21}^{(2)} & A_{22}^{(2)} \\
& & \ddots & \ddots \\
& & & \ddots & A_{11}^{(k)} & A_{12}^{(k)}
\end{pmatrix}.
\]

- interior domains can be factored in parallel
  $\implies$ great parallel performance!!

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A parallel hybrid linear solver
**Schur complement method:** with a block Gaussian elimination, we obtain

\[
\begin{pmatrix}
A_{11} & A_{12} \\
0 & S
\end{pmatrix}
\begin{pmatrix}
x_1 \\
x_2
\end{pmatrix} =
\begin{pmatrix}
I & 0 \\
-A_{21}A_{11}^{-1} & I
\end{pmatrix}
\begin{pmatrix}
b_1 \\
b_2
\end{pmatrix},
\]

where \( S = A_{22} - A_{21}A_{11}^{-1}A_{12} \) is the Schur complement.

Hence, the solution to the linear system can be computed by

1. solving \( Sx_2 = b_2 - A_{21}A_{11}^{-1}b_1 \)
2. solving \( A_{11}x_1 = b_1 - A_{12}x_2 \)

Most of fill occurs in \( S \), while \( A_{11} \) is block diagonal.
**Hybrid method**: Schur complement method

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Hence, the solution to the linear system can be computed by

1. solving \( Sx_2 = b_2 - A_{21}A_{11}^{-1}b_1 \) by an iterative method.
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**Hybrid method**: Schur complement method

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Hence, the solution to the linear system can be computed by

1. solving \( Sx_2 = b_2 - A_{21}A_{11}^{-1}b_1 \) by an iterative method.
2. solving \( A_{11}x_1 = b_1 - A_{12}x_2 \) by a direct method.

Most of fill occurs in \( S \), while \( A_{11} \) is block diagonal.
**HIPS** (Hybrid Iterative Parallel Solver):

- **developed by P. Henon and Y. Saad, 2008.**
- **features:**
  - each interior domain is factored by a single processor, number of interior domains ≥ number of processors.
  - fill in ILU is allowed between separators adjacent to same domain.
- **advantage:**
  - time to compute the preconditioner scales well.
- **disadvantage:**
  - to run on many processors, many interior domains are needed, which results in slow or no convergence
    - large Schur complement and poor preconditioner (fill is restricted within small blocks).
Our objectives:

to overcome the limitations of HIPS;

- factor each interior domain using multiple processors
  \[\Rightarrow\text{two-level parallelization (each domains in parallel)}\]
  more processors with a fixed Schur complement.

- improve flexibility and robustness of the solver
  \[\Rightarrow\text{faster convergence to solve Schur complement system.}\]

- exploit state-of-the-art techniques
  \[\Rightarrow\text{superior parallel performance.}\]

  to provide the flexibility and robustness to solve
large-scale highly-indefinite systems on many processors!!
New implementation.

- exploiting state-of-the-art software.
  - PT-SCOTCH to extract interior domains.
  - SuperLU_DIST to factor each interior domain.
  - PETSc to solve the Schur complement system.

- flexible and robust Schur complement solution.
  - efficient & stable formulation of approx. Schur
    - sparsity to reduce operation count and communication.
    - preprocessing for numerical stability and sparsity.
    - load-balancing and comm. strategies for good parallel performance.
  - choice of different preconditioners and solvers
    - SuperLU_DIST, Phidal, or any preconditioner from PETSc.
    - any solvers from PETSc
Preliminary results: tdr455k with $n = 2,738,556$.  

- 1-level parallelization; one processor per domain.  
- 2-level parallelization; multiple processors per domains.  
  - 16 interior domains.  
  - Processors evenly distributed among interior domains.  
  - 16 processors to solve Schur complement system.

<table>
<thead>
<tr>
<th>doms</th>
<th>16</th>
<th>32</th>
<th>63</th>
<th>128</th>
<th>256</th>
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<td>itrs</td>
<td>11</td>
<td>15</td>
<td>15</td>
<td>17</td>
<td>16</td>
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</tbody>
</table>

- Hybrid solver scaled better than direct solver.  
- Convergence (GMRES) only slightly degrades with more domains.  
- HIPS required 150 iterations and took longer for 16 domains, and failed to converge within 1000 iterations for 32 domains.
Preliminary results: **tdr455k** with $n = 2,738,556$.

- large drop tolerances to reduce memory cost.
- **1-level parallelization:**
  
  $\#$ of processors = $\#$ of domains.

- 1-level needed more iterations with more processors.
- 2-level parallelization scaled better.
- working to improve the parallel performance.
Features of our implementation

- multiple processors to solve each interior systems:
  - more processors with fixed Schur complement.
- flexibility to solve Schur complement system:
  - choice of different preconditioners and iterative methods.
  - subset of processors to solve Schur complement system.
- better parallel performance than other state-of-the-art solvers.

Current work:

- improving scalability of parallel implementation.
  - improving load-balance to solve interior domains.
  - studying different communication strategies.
  - developing parallel ILU based on SuperLU_DIST.
- conducting further experimentation.
  - solving a large system on many processors.
  - profiling memory usage per processor.
- extending to solve complex systems.