Enhancing Scalability and Robustness of the Schur Complement Method Using Hierarchical Parallelism

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Solvers:
- TOPS (Towards Optimal Petascale Simulations)
- FASTMath (Frameworks, Algorithms, and Scalable Technologies for Mathematics)

Application partnership:
- CEMM (Center for Extended MHD Modeling, fusion energy)
- ComPASS (Community Petascale Project for Accelerator Science and Simulation)
OUTLINE OF THE TALK

- Hybrid solver based on Schur complement method
  - Software: **PDSLin** (Parallel Domain decomposition Schur complement Linear solver)

- Combinatorial problems in hybrid solver
  - Sparse triangular solution with sparse right-hand sides
  - K-way graph partitioning with multiple constraints

... Focusing on scalability issues.
Schur complement method

- a.k.a. iterative substructuring method or, non-overlapping domain decomposition

Divide-and-conquer paradigm . . .
- Divide entire problem (domain, graph) into subproblems (subdomains, subgraphs)
- Solve the subproblems
- Solve the interface problem (Schur complement)

Variety of ways to solve subdomain problems and Schur complement ... lead to a powerful poly-algorithm or hybrid solver framework
Algebraic view

1. Reorder into 2x2 block system, $A_{11}$ is block diagonal

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

2. Schur complement

\[
S = A_{22} - A_{21} A_{11}^{-1} A_{12} = A_{22} - (U_{11}^{-T} A_{21}^{-T} L_{11}^{-1}) = A_{22} - W \cdot G
\]

where $A_{11} = L_{11} U_{11}$

$S$ corresponds to interface (separator) variables, no need to form explicitly

3. Compute the solution

\[
(1) \quad x_2 = S^{-1} (b_2 - A_{21} A_{11}^{-1} b_1) \quad \leftarrow \text{iterative solver}
\]

\[
(2) \quad x_1 = A_{11}^{-1} (b_1 - A_{12} x_2) \quad \leftarrow \text{direct solver}
\]
Structural analysis view

- **Case of two subdomains**

  Substructure contribution: \( A^{(k)} = \begin{pmatrix} A_{ii}^{(k)} & A_{iI}^{(k)} \\ A_{Ii}^{(k)} & A_{II}^{(k)} \end{pmatrix} \)  
  
  \( i = "\text{interior}" \)  
  
  \( I = "\text{Interface}" \)

1. **Assembled block matrix** \( A = \begin{pmatrix} A_{ii}^{(1)} & A_{ii}^{(2)} & A_{iI}^{(1)} \\ A_{iI}^{(1)} & A_{ii}^{(2)} & A_{iI}^{(2)} \\ A_{II}^{(1)} & A_{II}^{(2)} & A_{II}^{(1)} + A_{II}^{(2)} \end{pmatrix} \)

2. **Perform direct elimination of** \( A^{(1)} \) **and** \( A^{(2)} \) **independently,**

   Local Schur complements: \( S^{(k)} = A_{II}^{(k)} - A_{iI}^{(k)} (A_{ii}^{(k)})^{-1} A_{iI}^{(k)} \)

   Assembled Global Schur complement \( S = S^{(1)} + S^{(2)} \)
Solving the Schur complement system

**SPD, conditioning property** [Smith/Bjorstad/Gropp’96]
For an SPD matrix, condition number of a Schur complement is no larger than that of the original matrix.

- S is SPD, much reduced in size, better conditioned, but denser, solvable with preconditioned iterative solver

**Two approaches to preconditioning S**

1. Global S (e.g., PDSLin [Yamazaki/L.’10], HIPS [Henon/Saad’08])
   - general algebraic preconditioner, e.g. ILU(S)
2. Local S (e.g. MaPHys [Giraud/Haidary/Pralet’09])
   - restricted preconditioner; more parallel
   - e.g., additive Schwarz preconditioner  \( S = S^{(1)} \oplus S^{(2)} \oplus S^{(3)} \ldots \)

\[
M = S^{(1)^{-1}} \oplus S^{(2)^{-1}} \oplus S^{(3)^{-1}} \ldots
\]
## Related work

<table>
<thead>
<tr>
<th>PDSLin (LBNL)</th>
<th>MaPHyS (INRIA/CERFACS)</th>
<th>HIPS (INRIA)</th>
</tr>
</thead>
</table>

**PDSLin**
- Uses **two levels of parallelization and load-balancing techniques** for tackling large-scale systems
- Provides a **robust** preconditioner for solving highly-indefinite or ill-conditioned systems

**On-going work:** comparison of PDSLin and MaPHyS [Yamazaki et al.]
Parallelization with serial subdomain

- No. of subdomains increases with increasing core count.
  - Schur complement size and iteration count increase

HIPS (serial subdomain) vs. PDSLin (parallel subdomain)
- M3D-C\(^1\), Extended MHD to model fusion reactor tokamak, 2D slice of 3D torus
- Dimension 801k, 70 nonzeros per row, real unsymmetric

<table>
<thead>
<tr>
<th>P</th>
<th>N(_S)</th>
<th>HIPS 1.0 sec (iter)</th>
<th>PDSLin sec (iter)</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>13k</td>
<td>284.6 (26)</td>
<td>79.9 (15)</td>
</tr>
<tr>
<td>32</td>
<td>29k</td>
<td>55.4 (64)</td>
<td>25.3 (16)</td>
</tr>
<tr>
<td>128</td>
<td>62k</td>
<td>--</td>
<td>17.1 (16)</td>
</tr>
<tr>
<td>512</td>
<td>124k</td>
<td>--</td>
<td>21.9 (17)</td>
</tr>
</tbody>
</table>
Parallelism – extraction of multiple subdomains

Partition adjacency graph of $|A| + |A^T|$

Multiple goals: reduce size of separator, balance size of subdomains
- nested dissection (e.g., PT-Scotch, ParMetis)
- k-way partition (preferred)

$$
\begin{pmatrix}
A_{11} & A_{12} \\
A_{21} & A_{22}
\end{pmatrix}
= 
\begin{pmatrix}
D_1 & & \\
& D_2 & \\
& & \ddots
\end{pmatrix}
\begin{pmatrix}
E_1 \\
E_2 \\
\vdots
\end{pmatrix}
+ 
\begin{pmatrix}
F_1 \\
F_2 \\
\vdots
\end{pmatrix}
\begin{pmatrix}
D_k \\
E_k \\
A_{22}
\end{pmatrix}
$$

Memory requirement: fill is restricted within
- “small” diagonal blocks of $A_{11}$, and
- ILU(S), maintain sparsity via numerical dropping
Graph partitioning

Generalized nested dissection [Lipton/Rose/Tarjan ’79]
- Top-down, divide-and-conquer, best for largest problems
- Parallel codes: ParMetis, PT-Scotch
- First level

Goal: find the smallest separator S at each level
- Multilevel schemes:
  - ParMetis [Karypis et al.], PT-Scotch [Pellegrini et al.], PaToh [Catalyurek et al.]
  - Spectral bisection [Simon et al. ´90-´95]
  - Geometric and spectral bisection [Chan/Gilbert/Teng ´94]
Ordering

- Permute all the separators to the end

$$\begin{bmatrix}
A_{11} & A_{12} \\
A_{21} & A_{22}
\end{bmatrix} =
\begin{bmatrix}
D_1 & E_1 \\
D_2 & E_2 \\
\vdots & \vdots \\
D_k & E_k
\end{bmatrix}
$$

Separator tree
Hierarchical parallelism

- **Multiple processors per subdomain**
  - One subdomain with 2x3 procs (e.g. SuperLU_DIST, MUMPS)

- **Advantages:**
  - Constant #subdomains, Schur size, and convergence rate, regardless of core count.
  - Need only modest level of parallelism from direct solver.
PDSLin software

**Parallel Domain decomposition Schur complement based Linear solver**
- C and MPI, with Fortran interface.
- Unsymmetric and symmetric, real and complex, multiple RHSs.

**Requires the following external packages:**
- parallel graph partitioning:
  - PT-Scotch ([http://labri.fr/perso/pelegrin/scotch](http://labri.fr/perso/pelegrin/scotch)), or
  - ParMetis ([http://glaros.dtc.umn.edu/gkhome/views/metis](http://glaros.dtc.umn.edu/gkhome/views/metis))
- subdomain solver options:
  - SuperLU ([http://crd.lbl.gov/~xiaoye/SuperLU](http://crd.lbl.gov/~xiaoye/SuperLU))
  - SuperLU_DIST or SuperLU_MT: two levels of parallelization
  - MUMPS
  - PDSLin
  - Inexact subdomain solution: ILU
- Schur complement solver options:
  - PETSc ([http://mcs.anl.gov/petsc/petsc-as](http://mcs.anl.gov/petsc/petsc-as))
  - SuperLU_DIST
PDSLin encompass Hybrid, Iterative, Direct

Options
(1) num_doms = 0
   Schur = A: Krylov
(2) FGMRES Inner-Outer:
   Subdomain: ILU
   Schur: Krylov

Options
(1) Subdomain: LU
   Schur: LU
   drop_tol = 0.0
(2) num_doms = 1
   Domain: LU

\[
\begin{pmatrix}
D_1 & E_1 \\
D_2 & E_2 \\
\vdots & \vdots \\
D_k & E_k \\
F_1 & F_2 & \ldots & F_k & A_{22}
\end{pmatrix}
\]
PDSLin vs. SuperLU_DIST

- **Cray XT4 at NERSC**
- **Matrix211**: extended MHD to model burning plasma
  - dimension = 801K, nonzeros = 56M, real, unsymmetric
  - PT-Scotch extracts 8 subdomains of size ≈ 99K, S of size ≈ 13K
  - SuperLU_DIST to factorize each subdomain, and compute preconditioner LU($\widetilde{S}$)
  - BiCGStab of PETSc to solve Schur system on 64 processors with residual < 10^{-12}, converged in 10 iterations

- Needs only 1/3 memory of direct solver
PDSLin for RF cavity (strong scaling)

- Cray XT4 at NERSC; used 8192 cores
- Tdr8cavity: Maxwell equations to model cavity of International Linear Collider
  - dimension = 17.8M, nonzeros = 727M
  - PT-Scotch extracts 64 subdomains of size ≈ 277K, S of size ≈ 57K
  - BiCGStab of PETSc to solve Schur system on 64 processors
    - with residual < $10^{-12}$, converged in 9 ~ 10 iterations

- Direct solver failed!
PDSLIn for largest system

Matrix properties:

- 3D cavity design in Omega3P, 3rd order basis function for each matrix element
- dimension = 52.7 M, nonzeros = 4.3 B (~80 nonzeros per row), real, symmetric, highly indefinite

Experimental setup:

- PT-Scotch extracts 128 subdomains of size ~410k
- SuperLU DIST factors each subdomain, computes preconditioner LU(\(\tilde{S}\)) of size 247k (32 cores)
- BiCGStab of PETSc to solve \(Sy = d\)

Performance:

- Fill-ratio (nnz(Precond.)/nnz(A)): ~ 250
- Using 2048 cores:
  - preconditioner construction: 493.1 sec.
  - solution: 108.1 second (32 iterations)
Combinatorial problems

[ Yamazaki, L., Rouet, Ucar ]
Computing approximate Schur preconditioner

Combinatorial problems . . .

- **Sparse triangular solution with many sparse RHS**
  
  \[ S = A_{22} - \sum_{l} (U_l^{-T} F_l^T)^T (L_l^{-1} E_l), \quad \text{where} \quad D_l = L_l U_l \]

- **Sparse matrix–matrix multiplication**
  
  \[ \tilde{G} \leftarrow \text{sparsify}(G, \sigma_1); \quad \tilde{W} \leftarrow \text{sparsify}(W, \sigma_1) \]
  
  \[ T^{(p)} \leftarrow \tilde{W}^{(p)} \times \tilde{G}^{(p)} \]
  
  \[ \hat{S}^{(p)} \leftarrow A_{22}^{(p)} - \sum_q T^{(q)}(p); \quad \hat{S} \leftarrow \text{sparsify}(\hat{S}, \sigma_2) \]

- **K-way graph partitioning with multiple objectives**
  
  - Small separator
  
  - Similar subdomains
  
  - Similar connectivity
1. Sparse triangular solution with sparse RHS

- RHS vectors $E_\ell$ and $F_\ell$ are sparse (e.g., about 20 nnz per column); There are many RHS vectors (e.g., $O(10^4)$ columns)

![Diagram showing $L_\ell$ and $\hat{E}_\ell$](image)

**Blocking the RHS vectors**

- Reduce number of calls to the symbolic routine and number of messages, and improve read reuse of the LU factors
  - Achieved over 5x speedup
- Zeros must be padded to fill the block
Sparse triangular solution with sparse RHSs

- Combinatorial question: Reorder columns of $E_\ell$ to maximize structural similarity among the adjacent columns.

- Where are the fill-ins?

**Path Theorem** [Gilbert’94] Given the elimination tree of $D_\ell$, fill will be generated in $G_\ell$ at the positions associated with the nodes on the path from nodes of the nonzeros in $E_\ell$ to the root.

![Diagram of elimination tree and fill-ins](image)

Path from nodes of nonzeros in $E_\ell$ to the root:

- Paddded zeros: 24
Sparse triangular solution … postordering

- Postorder-conforming ordering of the RHS vectors
  - Postorder the elimination tree
  - Permute the columns of $E_1$ such that the row indices of the first nonzeros are in ascending order
- **Increased overlap** of the paths to the root, **fewer** padded zeros
- 20 – 40% reduction in solution time . . . improved over ND.
Sparse triangular solution … further optimization

- Define a cost function that measures the dissimilarity of the sparsity pattern within a partition.

- Reordering based on a hypergraph partitioning model which minimizes the cost function above.

- Led to additional 10% reduction in time.
2. K-way subdomain extraction

Problem with ND:
Imbalance in separator size at different branches $\rightarrow$ Imbalance in subdomain size

Alternative: directly partition into K parts, meet multiple constraints:

1. Compute k-way partitioning $\rightarrow$ balanced subdomains
2. Extract separator $\rightarrow$ balanced connectivity
Experimenting several heuristics

**Direct partition**
1. Scotch: k-way edge partition
   - Parts have similar size; minimize number of edge cuts
2. Form edge-induced subgraph
   - Two end-points form wide vertex separator
   - Find smaller vertex separator via minimal vertex cover

**Recursive hypergraph partitioning**

**Results**
+ improved balance of subdomains and interface
  - larger Schur complement & interfaces
  → total time improved a little
Final remarks

- Direct solvers can scale to 1000s cores

- Domain-decomposition type of hybrid solvers can scale to 10,000s cores
  - Can maintain robustness too

- Expect to scale more with low-rank structured factorization preconditioner
Extra Slides
Application 1: Burning plasma for fusion energy

- DOE SciDAC project: Center for Extended Magnetohydrodynamic Modeling (CEMM), PI: S. Jardin, PPPL

- Develop simulation codes to predict microscopic MHD instabilities of burning magnetized plasma in a confinement device (e.g., tokamak used in ITER experiments).
  - Efficiency of the fusion configuration increases with the ratio of thermal and magnetic pressures, but the MHD instabilities are more likely with higher ratio.

- Code suite includes M3D-C$^1$, NIMROD

  - At each $\phi = $ constant plane, scalar 2D data is represented using 18 degree of freedom quintic triangular finite elements $Q_{18}^1$

  - Coupling along toroidal direction

(S. Jardin)
Application 2: Accelerator cavity design

- DOE SciDAC: Community Petascale Project for Accelerator Science and Simulation (ComPASS), PI: P. Spentzouris, Fermilab
- Development of a comprehensive computational infrastructure for accelerator modeling and optimization
- RF cavity: Maxwell equations in electromagnetic field
- FEM in frequency domain leads to large sparse eigenvalue problem; needs to solve shifted linear systems

\[
(K_0 - \sigma^2 M_0) x = M_0 b
\]

\[
(K_0 + i \sigma W - \sigma^2 M_0) x = b
\]