Some investigations of an hybrid solver on unsymmetric and indefinite problems

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joint work with

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Outline

1 Motivations

2 Algebraic Additive Schwarz preconditioner
   - Introduction
   - Description of the preconditioner
   - Variant of Additive Shwarz preconditioner $M_{AS}$

3 Parallel numerical experiments
   - Numerical scalability
Outline

1. Motivations

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3. Parallel numerical experiments
   - Numerical scalability
Solution of very Large/Huge ill-conditioned linear systems

- Such problems can require thousands of CPU-hours and many Gigabytes of memory
- Direct solvers:
  - Robust and usually do not fail
  - Memory and computational costs grow nonlinearly
- Iterative solvers:
  - Reduce memory requirements
  - They may fail to converge
  - Typically implemented with preconditioning to accelerate convergence

In an effort to reduce these requirements, a parallel mechanism for combining solvers is needed
Goal

Develop a robust scalable parallel hybrid direct/iterative linear solvers

- Exploit the efficiency and robustness of the sparse direct solvers
- Take advantage of the natural scalable parallel implementation of iterative solvers
- Develop robust parallel preconditioners for iterative solvers

Non-overlapping domain decomposition

- Natural approach for PDE’s
- Extend to general sparse matrices
- Partition the problem into subdomains, subgraphs
- Use a direct solver on the subdomains
- Robust preconditioned iterative solver on interface
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Hybrid solver on unsymmetric and indefinite systems
Background

Algebraic splitting and block Gaussian elimination: N sub-domains case

\[
\begin{pmatrix}
A_{I_1I_1} & \cdots & 0 & A_{I_1\Gamma_1} \\
\vdots & \ddots & \vdots & \vdots \\
0 & \cdots & A_{I_NI_N} & A_{I_N\Gamma_N} \\
A_{\Gamma_1I_1} & \cdots & A_{\Gamma_NI_N} & A_{\Gamma\Gamma}
\end{pmatrix}
\begin{pmatrix}
u_{I_1} \\
\vdots \\
u_{I_N} \\
u_{\Gamma}
\end{pmatrix} =
\begin{pmatrix}
f_{I_1} \\
\vdots \\
f_{I_N} \\
f_{\Gamma}
\end{pmatrix}
\]

\[Su_{\Gamma} = \left( \sum_{i=1}^{N} R_{\Gamma_i}^T S^{(i)} R_{\Gamma_i} \right) u_{\Gamma} = f_{\Gamma} - \sum_{i=1}^{N} R_{\Gamma_i}^T A_{\Gamma_iI_i} A_{I_iI_i}^{-1} f_{I_i}
\]

where

\[S^{(i)} = A_{\Gamma_i\Gamma_i}^{(i)} - A_{\Gamma_iI_i} A_{I_iI_i}^{-1} A_{I_i\Gamma_i}
\]
Additive Schwarz preconditioner

**Motivations**

- Algebraic Additive Schwarz preconditioner
- Parallel numerical experiments

**Introduction**
- Description of the preconditioner
- Variant of Additive Shwarz preconditioner $M_{AS}$

**Additive Schwarz preconditioner** [Carvalho, Giraud, Meurant, 01]

**Preconditioner properties**

\[ M_{AS} = \sum_{i=1}^{\text{#domains}} R_i^T (\bar{S}^{(i)})^{-1} R_i \]

\[
\bar{S}^{(i)} = \begin{pmatrix}
S_{mm} & S_{mg} & S_{mk} & S_{m\ell} \\
S_{gm} & S_{gg} & S_{gk} & S_{g\ell} \\
S_{km} & S_{kg} & S_{kk} & S_{k\ell} \\
S_{\ell m} & S_{\ell g} & S_{\ell k} & S_{\ell\ell}
\end{pmatrix}
\]

\[
S^{(i)} = \begin{pmatrix}
S_{mm}^{(i)} & S_{mg}^{(i)} & S_{mk}^{(i)} & S_{m\ell}^{(i)} \\
S_{gm}^{(i)} & S_{gg}^{(i)} & S_{gk}^{(i)} & S_{g\ell}^{(i)} \\
S_{km}^{(i)} & S_{kg}^{(i)} & S_{kk}^{(i)} & S_{k\ell}^{(i)} \\
S_{\ell m}^{(i)} & S_{\ell g}^{(i)} & S_{\ell k}^{(i)} & S_{\ell\ell}^{(i)}
\end{pmatrix}
\]

Assembled local Schur complement

\[ S_{mm} = \sum_{j \in \text{AJA}(m)} S_{mm}^{(j)} \]

local Schur complement

Hybrid solver on unsymmetric and indefinite systems
Parallel implementation for solving $Au = f$

- Each *subdomain* $A^{(i)}$ is handled by one *processor*

$$A^{(i)} \equiv \begin{pmatrix} A_{I_iI_i} & A_{I_i\Gamma_i} \\ A_{I_i\Gamma_i} & A_{\Gamma_i\Gamma_i} \end{pmatrix}$$

- Concurrent partial factorizations are performed on each processor to form the so called “local Schur complement”

$$S^{(i)} = A_{I_iI_i}^{(i)} - A_{I_i\Gamma_i}A_{\Gamma_iI_i}^{-1}A_{I_i\Gamma_i}$$

- The reduced system $Sx = b$ is solved using a distributed Krylov solver
  - One matrix vector product per iteration each processor compute $S^{(i)}(x^{(i)})^k = (y^{(i)})^k$
  - One local preconditioner apply $(S^{(i)})^{-1}(z^{(i)})^k = (r^{(i)})^k$
  - Local neighbor-neighbor communication per iteration
  - Dot products per iteration (reduction)

- Compute simultaneously the solution for the interior unknowns

$$A_{I_iI_i}u_{I_i} = f_{I_i} - A_{I_i\Gamma_i}u_{\Gamma_i}$$

Hybrid solver on unsymmetric and indefinite systems
Sparsification strategy

- Allow entries whose magnitude exceeds a "drop tolerance"

\[
\hat{s}_{k\ell} = \begin{cases} 
\bar{s}_{k\ell} & \text{if } \bar{s}_{k\ell} \geq \epsilon (|\bar{s}_{kk}| + |\bar{s}_{\ell\ell}|) \\
0 & \text{else}
\end{cases}
\]

Two-level preconditioner

- Domain based coarse space correction
- \[ M = M_{AS} + R_0^T A_0^{-1} R_0 \text{ where } A_0 = R_0 S R_0^T \]
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Computational framework

Target computer
- IBM-SP4 @ CERFACS (216 procs)
- Blue Gene @ CERFACS (2048 procs)
- System X @ VIRGINIA TECH (2200 procs)

Local direct solver: MUMPS [Amestoy, Duff, Koster, L’Excellent - 01]
- Main features
  - Parallel distributed multifrontal solver (F90, MPI)
  - Symmetric and Unsymmetric factorizations
  - Element entry matrices, distributed matrices
  - Efficient Schur complement calculation
  - Iterative refinement and backward error analysis
- Public domain: new version 4.7.3
  www.enseeiht.fr/apo/MUMPS - mumps@cerfacs.fr
Numerical scalability for 3D unsymmetric problems

\[-\text{div}(K \cdot \nabla \phi) + v \cdot \nabla \phi = f\]

**xy plan view of the circular velocity field**

**Heterogenous convection diffusion**

- Scaled experiments on constant subdomain size of about 15000 dof
- The computing time increases slightly when increasing # sub-domains
Numerical scalability for 3D unsymmetric problems

\[-\text{div}(K\cdot\nabla\phi) + \mathbf{v}\cdot\nabla\phi = f\]

xy plan view of the 4-area velocity field

Anisotropic Heterogenous convection diffusion

- Scaled experiments on constant subdomain size of about 15000 dof
- The computing time increases slightly when increasing # sub-domains
Numerical scalability for 3D unsymmetric problems

\[-\epsilon \text{div}(K \cdot \nabla \phi) + v \cdot \nabla \phi = f\]

- Scaled experiments on constant subdomain size of about 15000 dof
- Smaller $\epsilon$, harder the solution is
Parallel performance for 3D indefinite problems

S. Pralet, SAMTECH

Structural mechanic indefinite pb

Parallel Performance and Scalability

<table>
<thead>
<tr>
<th># processors</th>
<th>8</th>
<th>16</th>
<th>32</th>
<th>64</th>
</tr>
</thead>
<tbody>
<tr>
<td># iter Dense</td>
<td>59</td>
<td>85</td>
<td>106</td>
<td>156</td>
</tr>
<tr>
<td># iter Sparse $\xi = 10^{-6}$</td>
<td>59</td>
<td>85</td>
<td>108</td>
<td>157</td>
</tr>
<tr>
<td># iter Sparse $\xi = 5.10^{-6}$</td>
<td>60</td>
<td>91</td>
<td>114</td>
<td>162</td>
</tr>
<tr>
<td># iter Sparse $\xi = 5.10^{-5}$</td>
<td>70</td>
<td>104</td>
<td>131</td>
<td>191</td>
</tr>
</tbody>
</table>

Hybrid solver on unsymmetric and indefinite systems
Backward error history

- Dense and Sparse preconditioners behavior

3D indefinite Rouet problem

- Time = local direct factorisation + setup preconditioner + iterative loop
- Backward history on the Schur complement of a problem with $1.3 \times 10^6$ dof mapped on 16 processors
Parallel performance for 3D indefinite problems

Motivations
Algebraic Additive Schwarz preconditioner
Parallel numerical experiments

Numerical scalability

Parallel Performance and Scalability

Structural mechanic problem

S. Pralet, SAMTECH

Hybrid solver on unsymmetric and indefinite systems
Backward error history

- Dense and Sparse preconditioners behavior

**3D indefinite Fuselage problem**

- **Time** = local direct factorisation + setup preconditioner + iterative loop
- Backward history on the Schur complement of a problem with $6.5 \times 10^6$ dof mapped on 16 processors