Algebraic Domain Decomposition Methods for Darcy flow in heterogeneous media

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December 29, 2010

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Why Domain Decomposition Method ?

- The term Domain Decomposition has slightly different meaning to specialist within the discipline of PDEs.
 - process of distributing data among the processors
 - process of subdividing the solution of large linear system into smaller problem
- Ease of parallelization
 - parallel processing is one way to have a faster codes
 - new generation processors are parallel (multi cores)
- In some situation, the domain decomposition is natural
 - strong heterogeneous media
 - different physics in different subdomains

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State of the Arts

New Methods and Techniques Conclusion and Prospects

DDM vs. other methods



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DDM vs. other methods



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DDM vs. other methods



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New Methods and Techniques Conclusion and Prospects

Original Method



$$\begin{array}{rcl} -\Delta(u) &=& f & \mathrm{in} & \Omega \\ u &=& g & \mathrm{on} & \partial\Omega \end{array}$$

Alternating Schwarz Method

$$\begin{array}{rclrcl} -\Delta(u_1^{n+1}) &=& f & \text{in} & \Omega_1 & -\Delta(u_2^{n+1}) &=& f & \text{in} & \Omega_2 \\ u_1^{n+1} &=& g & \text{on} & \partial\Omega_1 \backslash \Gamma_1 & u_2^{n+1} &=& g & \text{on} & \partial\Omega_2 \backslash \Gamma_2 \\ u_1^{n+1} &=& u_2^n & \text{on} & \Gamma_1. & u_2^{n+1} &=& u_1^{n+1} & \text{on} & \Gamma_2. \end{array}$$

"As $n \to \infty$, $(u_1^n, u_2^n) \to (u_{sol|\Omega_1}^n, u_{sol|\Omega_2}^n)$, where u_{sol} is a solution of continuous problem [Schwarz, 1870]."

State of the Arts

New Methods and Techniques Conclusion and Prospects

Parallel Schwarz Method



$$\begin{array}{rcl} -\Delta(u) &=& f & \mathrm{in} & \Omega \\ u &=& g & \mathrm{on} & \partial\Omega \end{array}$$

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New Methods and Techniques Conclusion and Prospects

Drawbacks of original methods

Original algorithms:

- are parallel but converges slowly
- need overlap in order to converge
- convergence speed depend on size of overlap

Improvements:

- Schwarz methods as a precondition for Krylov methods
- more general interface conditions

All of them can be apply at the algebraic level !

Example: The condition number κ of operator A, preconditioned by \mathcal{P}_{as} i.e., ASM with the coarse grid correction, satisfies

$$\kappa(\mathcal{P}_{as}A) \leq C\left(1 + \frac{H}{\delta}\right),$$

where the constant C is independent of, H and $\delta.$

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New Methods and Techniques Conclusion and Prospects

Algebraic Formulation (Jacobi and Schwarz)

Lets consider a discretized problem which yields a linear system.

$$\begin{array}{rcl} -\Delta(u) &=& f & \text{in} & \Omega \\ u &=& g & \text{on} & \partial\Omega \end{array} \qquad \qquad AU = F$$

For the set of indices Ω partitioned into two sets Ω_1 and Ω_2 we have:

$$\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} U_1 \\ U_2 \end{bmatrix} = \begin{bmatrix} F_1 \\ F_2 \end{bmatrix}$$



The block-Jacobi algorithm reads:

$$\begin{bmatrix} U_1^{n+1} \\ U_2^{n+1} \end{bmatrix} = \begin{bmatrix} U_1^n \\ U_2^n \end{bmatrix} + \begin{bmatrix} A_{11}^{-1} & 0 \\ 0 & A_{22}^{-1} \end{bmatrix} \begin{pmatrix} \begin{bmatrix} F_1 \\ F_2 \end{bmatrix} - \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} U_1^n \\ U_2^n \end{bmatrix} \end{pmatrix}$$

It corresponding to solving a Dirichlet boundary value problem in each subdomain with Dirichlet data taken from the other one at the previous step \implies Schwarz method with minimal overlap.

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New Methods and Techniques Conclusion and Prospects

Preconditioned Krylov space

$$\underbrace{\begin{bmatrix} U_1^{n+1} \\ U_2^{n+1} \end{bmatrix}}_{\mathbf{u}_1^{n+1}} = \begin{bmatrix} U_1^n \\ U_2^n \end{bmatrix} + \begin{bmatrix} A_{11}^{-1} & 0 \\ 0 & A_{22}^{-1} \end{bmatrix} \begin{pmatrix} \begin{bmatrix} F_1 \\ F_2 \end{bmatrix} - \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} U_1^n \\ U_2^n \end{bmatrix} \end{pmatrix}}_{\mathbf{u}_{n+1} = \mathbf{u}_n + M^{-1}(\mathbf{f} - A\mathbf{u}_n)}$$

Let $\mathbf{r}_0 := M^{-1} (\mathbf{f} - A\mathbf{u}_0)$, we have (fixed point method):

$$\mathbf{u}_n = \sum_{i=0}^n \left(\mathbb{I} - M^{-1} A \right)^i \mathbf{r}_0 + \mathbf{u}_0$$

A preconditioned Krylov solve will generate an optimal solution $\mathbf{u}_n^{\mathcal{K}}$ in:

$$\mathcal{K}_m\left(M^{-1}A, \mathbf{r}_0\right) := \mathbf{u}_0 + \operatorname{SPAN}\left\{\mathbf{r}_0, M^{-1}A\mathbf{r}_0, \dots, (M^{-1}A)^{m-1}\mathbf{r}_0\right\}$$

where $\mathbf{u}_n \in \mathcal{K}_m$ but with "frozen" coefficients $\implies \mathbf{u}_n$ is less optimal then $\mathbf{u}_n^{\mathcal{K}}$.

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New Methods and Techniques Conclusion and Prospects

Modified Schwarz Method

Another improvement arise from usage of more general interface conditions for a non-overlapping ($\iff \alpha > 0$) decomposition [Lions, 1990]:



$$\begin{array}{rcl} -\Delta(u) &=& f & \mathrm{in} & \Omega \\ u &=& g & \mathrm{on} & \partial\Omega \end{array} \tag{1}$$

$$\begin{array}{rcl} \hline \textbf{Modified Schwarz Method} \\ & \begin{array}{rcl} -\Delta(u_1^{n+1}) &=& f & \text{in } \Omega_1 \\ & u_1^{n+1} &=& g & \text{on } \partial\Omega_1 \backslash \Gamma \\ & \left(\frac{\partial}{\partial n_1} + \alpha\right) (u_1^{n+1}) &=& \left(\frac{\partial}{\partial n_2} + \alpha\right) (u_n^{n+1}) & \text{on } \partial\Omega_1 \cap \overline{\Omega}_2 \\ & \begin{array}{rcl} -\Delta(u_2^{n+1}) &=& f & \text{in } \Omega_2 \\ & u_2^{n+1} &=& g & \text{on } \partial\Omega_2 \cap \partial\Gamma \\ & \left(\frac{\partial}{\partial n_2} + \alpha\right) (u_2^{n+1}) &=& \left(\frac{\partial}{\partial n_1} + \alpha\right) (u_n^{n+1}) & \text{on } \partial\Omega_2 \cap \overline{\Omega}_1 \end{array}$$

Optimal Choice

J. L. Lions:

"First of all, it is possible to replace the constants in the Robin condition by two proportional function on the interface, or even by local or nonlocal operators [Lions, 1990]."

F. Nataf, F. Rogier and E. de Sturler:

"The rate of convergence of Schwarz and Schur type algorithms is very sensitive to the choice of interface condition. The original Schwarz method is based on the use of Dirichlet boundary conditions. In order to increase the efficiency of the algorithm, it has been proposed to replace the Dirichlet boundary condition with more general boundary conditions. . . . It has been remarked that absorbing (or artificial) boundary conditions are a good choice. In this report, we try to clarify the question of the interface condition [Nataf et al., 1994]."

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Optimal Choice

The authors proved that use of non-local DtN (*Dirichlet to Neumann*) map (a.k.a. *Steklov-Poincaré*) as interface condition in problem (1) leads to (*exact*) convergence in two iterations.

Definition (DtN map)

Let

$$u_0: \Gamma_1 \to \mathbb{R}$$
$$\mathrm{DtN}_2(u_0) := \nabla v \cdot n_{2|\partial\Omega_1 \cap \overline{\Omega}_2},$$

where n_2 is the outward normal to $\Omega_2 \setminus \overline{\Omega}_1$, and v satisfies the following boundary value problem:

$$\mathcal{L}(v) = 0 \quad ext{in} \quad \Omega_2 \setminus \overline{\Omega}_1 \ v = 0 \quad ext{on} \quad \partial \Omega_2 \cap \partial \Omega \ v = u_0 \quad ext{on} \quad \partial \Omega_1 \cap \overline{\Omega}_2.$$

State of the Arts

New Methods and Techniques

Optimal Interface Condition at the matrix level



In order to write a "modified" Schwarz method we need to introduce two square matrixes S_1 and S_2 which acts on vector of the type U_{Γ} :

$$\begin{pmatrix} A_{11} & A_{1\Gamma} \\ A_{\Gamma 1} & A_{\Gamma\Gamma} + S_2 \end{pmatrix} \begin{pmatrix} U_1^{n+1} \\ U_{\Gamma,1}^{n+1} \end{pmatrix} = \begin{pmatrix} F_1 \\ F_{\Gamma} + S_2 U_{\Gamma,2}^n - A_{\Gamma 2} U_2^n \end{pmatrix}$$
$$\begin{pmatrix} A_{22} & A_{2\Gamma} \\ A_{\Gamma 2} & A_{\Gamma\Gamma} + S_1 \end{pmatrix} \begin{pmatrix} U_2^{n+1} \\ U_{\Gamma,2}^{n+1} \end{pmatrix} = \begin{pmatrix} F_2 \\ F_{\Gamma} + S_1 U_{\Gamma,1}^n - A_{\Gamma 1} U_1^n \end{pmatrix}$$

Lemma

If $A_{\Gamma\Gamma} + S_1 + S_2$ is invertible and problem (1) is well-posed. Then above algorithm converges to the solution of (1) $\implies U_i^{\infty} = U_i$ and $U_{\Gamma,1}^{\infty} = U_{\Gamma,2}^{\infty} = U_{\Gamma}.$

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Optimal Interface Condition at the matrix level

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Optimal choice

Taking $S_1 = -A_{\Gamma 1}A_{11}^{-1}A_{1\Gamma}$ and $S_2 = -A_{\Gamma 1}A_{22}^{-1}A_{2\Gamma}$ yields a convergence in two steps $\implies A_{\Gamma\Gamma} - A_{\Gamma i}A_{i\Gamma}^{-1}A_{i\Gamma}$ is a Schur complement.

The matrices S_1 and S_2 are full, therefore

they are costly to build
 the subdomain matrix is partially full

However it is possible to approximate them by sparse matrices e.g., via local Schur complement on successive reduced "outer" domain, which we call **patches** [Magoulès et al., 2006].

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New Methods and Techniques

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The matrices S_1 and S_2 are full, therefore

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New Methods and Techniques Conclusion and Prospects

Schwarz method vs. Many subdomains

It is well known that performance may deteriorate with large number of subdomains i.e., plateaus appear in the convergence of the Krylov methods.

They are due to the lack of a global exchange of information in the preconditioner.



 $\begin{array}{rcl} -\Delta(u) &=& f & \mathrm{in} & \Omega \\ u &=& g & \mathrm{on} & \partial\Omega \end{array}$

The mean value of the solution in domain Ω_i depends on the value of f on all subdomains.

A classical remedy: \implies coarse grid problem that couples all subdomains.

 can be incorporate as additional preconditioner preconditioning".

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New Methods and Techniques Conclusion and Prospects

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New Methods and Techniques Conclusion and Prospects

Two-level preconditioner

From an abstract point of view, all two-level preconditioners of the method consists of an arbitrary preconditioner M, combined with one or more matrices P and Q.

$$P := \mathbb{I} - AQ, \quad Q := ZE^{-1}Z^T, \quad E := Z^T AZ$$

Some properties:

- $PA = AP^T$ $A, M, P, Q \in \mathbb{R}^{n \times n}$ $Z \in \mathbb{R}^{n \times m}$ • $P^T Z = \mathbf{0}, P^T Q$
- $QA = \mathbb{I} P^T$, QAZ = Z, QAQ = Q

 $E \in \mathbb{R}^{m \times m}$. $m \ll n$

New Methods and Techniques Conclusion and Prospects

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The matrix Z consists of so-called projection vectors, whose columns span the projection space (More detail in [Tang et al., 2009]).

Example: $\mathcal{P}_{AD} := M^{-1} + Q, \ \mathcal{P}_{BNN} := P^T M^{-1} P + Q, \ \mathcal{P}_{A-DEF} := P^T M^{-1} + Q$

What we know so far?

Schwarz methods:

- are very suitable for parallel computing
- are easy to use at the algebraic level
 - and its iterative process can by accelerated by Krylov methods
- they also "work" with general interface conditions
 - for which we know "optimal" choice
- we can modify interface conditions at the algebraic level
- in case of many subdomains, we can incorporate Schwarz preconditioner with the coarse grid correction
 - in order to construct two-level preconditioner

New Methods and Techniques

ADDMlib - parallel library

ADDMIib - Algebraic Domain Decomposition Methods (library)

- carefully design object oriented library
- written in modern C++ (Boost + STL)
- provides (via MPI) many of the mechanism needed within parallel application code
 - parallel vectors and sparse matrices in several sparse formats
- we put stress on:
 - easiness of implementing preconditioners of DDM type
 - Krylov subspace methods (GMRES,FGMRES,BiCGstab)
- it provides convenient interface for chosen functionality from other libraries like *METIS*, *SCOTCH* or *PETSc*



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ADDMlib - parallel library



Figure: DDMVector structure and its division into Partial Vectors according to decomposition of domain Ω .

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ADDMlib - parallel library



Figure: Decomposition of global linear system into Partial Vectors and Operators (very similar idea introduced independently in [Buluc et al., 2009]).

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Figure: Decomposition of global linear system into Partial Vectors and Operators (very similar idea introduced independently in [Buluc et al., 2009]).

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ADDMlib - parallel library



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Partitioning

But how to subdivide and map data into processors ?

- in arbitrary fashion
- or we can use adjacency graph partitioners (SCOTCH, METIS)

Definition (Graph Partitioning)

For a general sparse linear system whose adjacency graph is G = (V, E), the k-way graph partitioning problem is defined as follows: given a graph G = (V, E) with |V| = n, partition V into k subsets, V_1, V_2, \ldots, V_k such that $V_i \cap V_j = \emptyset$ for $i \neq j$, $|V_i| = n/k$, and $\cup_i V_i = V$, and the number of edges of E whose incident vertices belong to different subset is minimized.

During our experiments we have noticed that the way how the adjacency graph is partitioned has strong influence on overall performance of algebraic DDM.

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During our experiments we have noticed that the way how the adjacency graph is partitioned has strong influence on overall performance of algebraic DDM.

Partitioning with weights

There is a certain number of problems for which "smart" partitioning can increase robustness (e.g., anisotropic problems)

Is it possible to extract algebraically some information about physical properties of the problem to solve, and use them to obtain better partition ?

... yes we can define weights for edges of adjacency graph using values of the underlaying matrix using following formula adapted from AMG methods (see for example [Stüben, 2001])

Automatic weight labelling

$$c = \left\lfloor \left(\frac{|a_{ij}|}{|a_{ii}| + |a_{jj}|} \times \gamma_{const} \right) \right\rfloor$$

 $\lfloor x \rfloor$ is the floor function rounds the element x to the nearest integer toward minus infinity and γ_{const} is an arbitrary constant.

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Partitioning with weights - Numerical Experiment 1

Let us consider following, anisotropic problem: $-\kappa\Delta(\mathbf{u}) = f$, discretized (FreeFem++) on 2D unit square in size $N_x \times N_y$, where $N_x = N_y = 128$

$$\kappa = \begin{bmatrix} \kappa_{xx} & 0\\ 0 & \kappa_{yy} \end{bmatrix} = \begin{bmatrix} 1 \times 10^{-6} & 0\\ 0 & 1 \end{bmatrix}$$



Figure: a

Figure: b

Figure: c

Figure: d



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Partitioning with weights - Numerical Experiment 2





State of the Arts

New Methods and Techniques

Conclusion and Prospects

Partitioning with weights - real test case



nparts	nrows	nnz
32	49,572	480,612



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Partitioning with weights - real test case



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New Methods and Techniques

Conclusion and Prospects

Partitioning with weights - real test case (ALL)



Cost of one iteration and time of partitioning is about the same in both cases ${\tt !!}$

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New Methods and Techniques

Conclusion and Prospects

Partitioning with weights - real test case (ALL)



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State of the Arts

New Methods and Techniques Conclusion and Prospects

Enlarge overlap = algebraically *inflate* operator

 $\mathsf{Bigger} \text{ overlap } \implies \mathsf{faster} \text{ convergence } !!$



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New Methods and Techniques

Conclusion and Prospects

Enlarge overlap = algebraically *inflate* operator

Before inflation



Γ	$A_{1_i1_i}$	$A_{1_i\Gamma_1^2}$	0	0	0	0	0]	U_{1_i}		F_{1_i}
	$A_{\Gamma_1^2 1_i}$	$A_{\Gamma_1^2\Gamma_1^2}$	0	$A_{\Gamma_1^2\Gamma_2^1}$	0	0	0	$U_{\Gamma_1^2}$		$F_{\Gamma_1^2}$
-	0	0	$A_{2_i2_i}$	$A_{2_i\Gamma_2^1}$	$A_{2_i\Gamma_2^3}$	0	0	U_{2_i}		$\overline{F_{2_i}}$
	0	$A_{\Gamma_2^1\Gamma_1^2}$	$A_{\Gamma_2^1 2_i}$	$A_{\Gamma_2^1\Gamma_2^1}$	0	0	0	$U_{\Gamma_2^1}$	=	$F_{\Gamma_2^1}$
	0	0	$A_{\Gamma_2^3 2_i}$	0	$A_{\Gamma^3_2\Gamma^3_2}$	0	$A_{\Gamma^3_2\Gamma^2_3}$	$U_{\Gamma_2^3}$		$F_{\Gamma_2^3}$
	0	0	0	0	0	$A_{3_i 3_i}$	$A_{3_i\Gamma_3^2}$	U_{3_i}		F_{3_i}
L	0	0	0	0	$A_{\Gamma^2_3\Gamma^3_2}$	$A_{\Gamma_3^2 3_i}$	$A_{\Gamma^2_3\Gamma^2_3}$	$U_{\Gamma_3^2}$		$F_{\Gamma_3^2}$

New Methods and Techniques

Conclusion and Prospects

Enlarge overlap = algebraically *inflate* operator

After inflation



$A_{1_i1_i}$	$A_{1_i\Gamma_1^2}$	0	0	0	0	0	0	0	0	0 -
$A_{\Gamma_1^2 1_i}$	$A_{\Gamma_1^2\Gamma_1^2}$	$A_{\Gamma_1^2\Gamma_2^1}$	0	0	0	0	0	0	0	0
0	$A_{\Gamma_2^1\Gamma_1^2}$	$A_{\Gamma_2^1\Gamma_2^1}$	$A_{\Gamma_2^1 2_i}$	0	0	0	0	0	0	0
0	0	0	$A_{2_i2_i}$	$A_{2_i\Gamma_2^1}$	$A_{2_i\Gamma_2^3}$	0	0	0	0	0
0	0	0	$A_{\Gamma_2^1 2_i}$	$A_{\Gamma_2^1\Gamma_2^1}$	0 -	$A_{\Gamma^1_2\Gamma^2_1}$	0	0	0	0
0	0	0	$A_{\Gamma_2^3 2_i}$	Õ	$A_{\Gamma^3_2\Gamma^3_2}$	Õ	$A_{\Gamma^3_2\Gamma^2_2}$	0	0	0
$A_{\Gamma_1^2 1_i}$	0	0	0	$A_{\Gamma_1^2\Gamma_2^1}$	Ő	$A_{\Gamma^2_1\Gamma^2_1}$	Õ	0	0	0
0	0	0	0	0	$A_{\Gamma^2_3\Gamma^3_2}$	0	$A_{\Gamma^2_3\Gamma^2_3}$	$A_{\Gamma^2_3 3_i}$	0	0
0	0	0	0	0	0	0	0	$A_{3_{i}3_{i}}$	$A_{3_i\Gamma_3^2}$	0
0	0	0	0	0	0	0	0	$A_{\Gamma^2_3 3_i}$	$A_{\Gamma^2_3\Gamma^2_3}$	$A_{\Gamma^2_3\Gamma^3_2}$
0	0	0	$A_{\Gamma_2^3 2_i}$	0	0	0	0	0	$A_{\Gamma^3_2\Gamma^2_3}$	$A_{\Gamma_2^3\Gamma_2^3}$

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New Methods and Techniques

Conclusion and Prospects

Inflation vs Computational Time

Matrix L3D4x4x16n10.mtx

nparts	nrows	nnz
256	270,641	3,941,521









New Methods and Techniques Conclusion and Prospects

Modified Schwarz Method

New interface condition \implies additional augmented matrixes defined on the interface between sub-domains.

$A_{1_i1_i}$	$A_{1_i\Gamma_1^2}$	0	0	0	0	0	0	0	0	0 7
$A_{\Gamma_1^2 1_i}$	$A_{\Gamma_1^2\Gamma_1^2}$	$A_{\Gamma_1^2\Gamma_2^1}$	0	0	0	0	0	0	0	0
0	$A_{\Gamma_2^1\Gamma_1^2}$	$A_{\Gamma_2^1\Gamma_2^1} + S_2^1$	$A_{\Gamma_2^1 2_i}$	$-S_{2}^{1}$	0	0	0	0	0	0
0	0	0	$A_{2_i 2_i}$	$A_{2_i\Gamma_2^1}$	$A_{2_i\Gamma_2^3}$	0	0	0	0	0
0	0	0	$A_{\Gamma_2^1 2_i}$	$A_{\Gamma_2^1\Gamma_2^1}$	0	$A_{\Gamma^1_2\Gamma^2_1}$	0	0	0	0
0	0	0	$A_{\Gamma_{2}^{3}2_{i}}$	Õ	$A_{\Gamma^3_2\Gamma^3_2}$	Õ	$A_{\Gamma_2^3\Gamma_3^2}$	0	0	0
$A_{\Gamma_1^2 1_i}$	$-S_{1}^{2}$	0	Ő	$A_{\Gamma_1^2\Gamma_2^1}$	Õ	$A_{\Gamma_{1}^{2}\Gamma_{1}^{2}}+S_{1}^{2}$	Õ	0	0	0
0	0	0	0	0	$A_{\Gamma^2_3\Gamma^3_2}$	Ô	$A_{\Gamma^2_3\Gamma^2_3} {+} S^2_3$	$A_{\Gamma^2_3 3_i}$	$-S_{3}^{2}$	0
0	0	0	0	0	0	0	0	$A_{3_{i}3_{i}}$	$A_{3_i\Gamma_3^2}$	0
0	0	0	0	0	0	0	0	$A_{\Gamma_3^2 3_i}$	$A_{\Gamma^2_3\Gamma^2_3}$	$A_{\Gamma_3^2\Gamma_2^3}$
0	0	0	$A_{\Gamma_2^3 2_i}$	0	$-S_{2}^{3}$	0	0	0	$A_{\Gamma^3_2\Gamma^2_3}$	$A_{\Gamma_{2}^{3}\Gamma_{2}^{3}} + S_{2}^{3}$

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New Methods and Techniques

Conclusion and Prospects

Modified Schwarz Method - Optimal Interface Conditions



Optimal choice for two domain case

The choice of S_1 and S_2 can be "adjusted" in such a way that Schur complements appears in inflated operator \widetilde{A} i.e.

$$S_1^{opt} = -A_{2_{\Gamma}2_i}A_{2_i2_i}^{-1}A_{2_i2_i}$$

$$S_2^{opt} = -A_{1_{\Gamma}1_i}A_{1_i1_i}^{-1}A_{1_i1_r}$$

is optimal, and the ASM in form of preconditioner in an iterative Krylov solver, converges in two steps.

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New Methods and Techniques Conclusion and Prospects

Optimal Interface Conditions Approximation

For a sake of simplicity we consider only two subdomains and we focus on domain Ω_1 which we simply denote by 1 and its inflated counterpart by $\widetilde{1}$.



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New Methods and Techniques Conclusion and Prospects

Optimal Interface Conditions Approximation - General Case

What about general case (2 < N - subdomains)?



Diagonal Approximation

GOAL: approximate optimal interface conditions by a sparse matrix keeping some filtering properties.

$$S^{opt}_{\widetilde{\Gamma}_1\widetilde{\Gamma}_1} := -A_{\widetilde{\Gamma}_1\widetilde{1}_c} A^{-1}_{\widetilde{1}_c\widetilde{1}_c} A_{\widetilde{1}_c\widetilde{\Gamma}_1}$$

More precisely we seek an approximation to $S^{opt}_{\widetilde{\Gamma}_1\widetilde{\Gamma}_1}$ in form:

The optimal interface conditions approximation

$$S^{\approx}_{\widetilde{\Gamma}_1\widetilde{\Gamma}_1} := -A_{\widetilde{\Gamma}_1\widetilde{1}_c}\beta_{\widetilde{1}_c\widetilde{1}_c}A_{\widetilde{1}_c\widetilde{\Gamma}_1}$$

such that, the optimality condition is verified on the vector $V_{\widetilde{\Gamma}_1}$

$$-A_{\widetilde{\Gamma}_1\widetilde{1}_c}\beta_{\widetilde{1}_c\widetilde{1}_c}A_{\widetilde{1}_c\widetilde{\Gamma}_1}V_{\widetilde{\Gamma}_1}=S^{opt}_{\widetilde{\Gamma}_1\widetilde{\Gamma}_1}V_{\widetilde{\Gamma}_1}$$

where V is a harmonic vector i.e.,

$$A_{\widetilde{1}_c\widetilde{1}_c}V_{\widetilde{1}_c} + A_{\widetilde{1}_c\widetilde{\Gamma}_1}V_{\widetilde{\Gamma}_1} = 0$$

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Sparse matrix $\beta_{\tilde{1},\tilde{1},\tilde{1}}$

If V is a harmonic vector in $\widetilde{1}_c,$ we take $\beta_{\widetilde{1}_c\widetilde{1}_c}$ to be a diagonal matrix defined by

$$\beta_{\tilde{1}_{c}\tilde{1}_{c}} \text{ operator}$$
$$\beta_{\tilde{1}_{c}\tilde{1}_{c}} := diag\left(-V_{\tilde{1}_{c}}./A_{\tilde{1}_{c}\tilde{\Gamma}_{1}}V_{\tilde{\Gamma}_{1}}\right)$$

and
$$\beta_{\tilde{1}_c\tilde{1}_c} = 0$$
 otherwise.

"./" - element wise division

$$\begin{bmatrix} v_1 \\ \vdots \\ v_n \end{bmatrix} \cdot / \begin{bmatrix} w_1 \\ \vdots \\ w_n \end{bmatrix} = \begin{bmatrix} v_1/w_1 \\ \vdots \\ v_n/w_n \end{bmatrix}$$

Harmonic Vector - Facts

- Due to the block preconditioner M^{-1} (the Schwarz method) the vectors in the *Krylov* space $\mathcal{K}_m(\widetilde{M}^{-1}\widetilde{A}, r_0)$ are sub-domain wise harmonic.
- Many iterative methods use Krylov space for computation (selected) eigenvalues.
- Our choice of harmonic vector is an approximated eigenvector of $\widetilde{M}^{-1}\widetilde{A}$ assosiated with the smallest eigenvalue λ (we use Krylov subspaces created via GMRES).

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- **1** The computational kernel of GMRES is the Arnoldi process which computes the orthonormal basis W_m for the Krylov subspace $\mathcal{K}_m(\widetilde{M}^{-1}\widetilde{A}, r_0)$.
- 2 Since the Arnoldi basis is orthonormal, $W_m = (w_1 \ w_2 \ \dots \ w_m)$ is an orthogonal matrix $(W_m \in \mathbb{R}^{n \times m})$.
- 3 In the orthogonalisation process the scalars h_{ij} are computed so that the square upper *Hessenberg* matrix $H_m \in \mathbb{R}^{m \times m}$ satisfies the fundamental relation:

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(3) The eigenvalues of H_m are called Ritz values and they approximate the eigenvalues of $\widetilde{M}^{-1}\widetilde{A}$.

if z_{\star} is an chosen eigenvector of H_m , then $\mathcal{V}_{\star} = W_m z_{\star}$ is almost an eigenvector of $\widetilde{M}^{-1}\widetilde{A}$, for the same eigenvalue λ i.e.,

$$\widetilde{M}^{-1}\widetilde{A}\mathcal{V}_{\star} \simeq W_m H_m W_m^H W_m z_{\star} = = W_m H_m z_{\star} = = W_m \lambda z_{\star} = \lambda \mathcal{V}_{\star}$$

In practice a specific Lapack procedure can be used to compute the eigenelements of H_m .

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State of the Arts

New Methods and Techniques Conclusion and Prospects

Numerical Experiments with EDOIC

Two sub-domain (complex) case:

$$\begin{cases} \left(\eta(x,y) - div(\kappa(x,y)\overrightarrow{\nabla})\right)u(x,y) &= f(x,y) \quad \text{in} \quad \Omega\\ u(x,y) &= 0 \quad \text{on} \quad \partial\Omega_D\\ \frac{\partial u}{\partial n} &= 0 \quad \text{on} \quad \partial\Omega_N \end{cases}$$



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New Methods and Techniques Conclusion and Prospects

Numerical Experiments with EDOIC



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New Methods and Techniques Conclusion and Prospects

Numerical Experiments with EDOIC



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New Methods and Techniques

Conclusion and Prospects

Numerical Experiment (fixed size problem)

Fixed size problem $n_x = n_y = 50$



(a)
$$M_x = M_y = 2$$



(b) $M_x = M_y = 3$

100100100100100100100100100100100100100	
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1001101101101100100100 10011011011011011	_
An an an analog and an	

(c)
$$M_x = M_y = 4$$





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New Methods and Techniques Conclusion and Prospects

Two-level preconditioner

PROBLEM: Convergence of the Schwarz method deteriorates with increasing number of subdomains.

SOLUTION: "Remove" smallest eigenvalues that slow down the Schwarz method.

It leads us to construction of two-level preconditioner using

$$P := \mathbb{I} - A \left(Z E^{-1} Z^T \right) \quad E := Z^T A Z$$

which are common ingredients of the coarse grid, deflation and AMG preconditioners (see [Tang et al., 2009]).

An effective two-level preconditioner is highly dependent on the choice of coarse grid subspace $Z \in \mathbb{R}^{n \times m}$.

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How to choose Z ?

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New Methods and Techniques Conclusion and Prospects

Coarse grid correction for smooth problems

For a Poisson like problem, Nicolaides proposed [Nicolaides, 1987]:



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New Methods and Techniques Conclusion and Prospects

Coarse grid correction for smooth problems

For a Poisson like problem, Nicolaides proposed [Nicolaides, 1987]:



In deflation techniques Z consists of eigenvectors or approximations of eigenvectors (which we know how to find: $\mathcal{V}_{\star}=W_m z_{\star})$

$$Z^{\star} := [\mathcal{V}_{1} \mathcal{V}_{2} \cdots \mathcal{V}_{n_{\mathcal{V}}}] = \begin{bmatrix} [\mathcal{V}_{1}]_{\widetilde{D}_{\Omega_{1}}} & [\mathcal{V}_{2}]_{\widetilde{D}_{\Omega_{1}}} & \cdots & [\mathcal{V}_{n_{\mathcal{V}}}]_{\widetilde{D}_{\Omega_{1}}} \\ [\mathcal{V}_{1}]_{\widetilde{D}_{\Omega_{2}}} & [\mathcal{V}_{2}]_{\widetilde{D}_{\Omega_{2}}} & \cdots & [\mathcal{V}_{n_{\mathcal{V}}}]_{\widetilde{D}_{\Omega_{2}}} \\ \vdots & \vdots & & \vdots \\ [\mathcal{V}_{1}]_{\widetilde{D}_{\Omega_{N}}} & [\mathcal{V}_{2}]_{\widetilde{D}_{\Omega_{N}}} & \cdots & [\mathcal{V}_{n_{\mathcal{V}}}]_{\widetilde{D}_{\Omega_{N}}} \end{bmatrix}$$

We can apply a part wise spliting to Z^* in order to construct a coarse subspace similar in structure to one proposed by Nicolaides.

Our choice of Z

In deflation techniques Z consists of eigenvectors or approximations of eigenvectors (which we know how to find: $V_{\star} = W_m z_{\star}$)

Н	С	oarse (grid sı	ıbs	pace Z	$\in \mathbb{R}^{n}$	$\times (n_v \times$	N)					
		$[\mathcal{V}_1]_{\widetilde{D}_{\Omega_1}}$	$[\mathcal{V}_2]_{\widetilde{D}_{\Omega_1}}$		$[\mathcal{V}_{n_{\mathcal{V}}}]_{\widetilde{D}_{\Omega_{\mathcal{V}}}}$	0	0		0		0	0	 0]
7		01	0		0	$[\mathcal{V}_1]_{\widetilde{D}\Omega_2}$	$[\mathcal{V}_2]_{\widetilde{D}\Omega_2}$	•••	$[\mathcal{V}_{n_{\mathcal{V}}}]_{\widetilde{D}_{\Omega_2}}$	•••	0	0	 0
Z :=	:=	÷	÷		:	÷	:		÷		÷	÷	:
		0	0		0	0	0	•••	0	•••	$[\mathcal{V}_1]_{\widetilde{D}_{\Omega_N}}$	$[\mathcal{V}_2]_{\widetilde{D}_{\Omega_N}}$	 $[\mathcal{V}_{n\nu}]_{\widetilde{D}\Omega_N}$

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$$\begin{array}{c} \textbf{Coarse grid subspace } Z \in \mathbb{R}^{n \times (2 \times 3)} \\ Z^{\star} := \begin{bmatrix} [\mathcal{V}_1]_{\tilde{D}_{\Omega_1}} & [\mathcal{V}_2]_{\tilde{D}_{\Omega_1}} \\ [\mathcal{V}_1]_{\tilde{D}_{\Omega_2}} & [\mathcal{V}_2]_{\tilde{D}_{\Omega_2}} \\ [\mathcal{V}_1]_{\tilde{D}_{\Omega_3}} & [\mathcal{V}_2]_{\tilde{D}_{\Omega_3}} \end{bmatrix} \rightarrow \begin{bmatrix} [\mathcal{V}_1]_{\tilde{D}_{\Omega_1}} & [\mathcal{V}_2]_{\tilde{D}_{\Omega_1}} \\ & & & & & & \\ \end{bmatrix} = Z \end{array}$$

We can apply a part wise spliting to Z^* in order to construct a coarse subspace similar in structure to one proposed by Nicolaides.

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New Methods and Techniques Conclusion and Prospects

Our choice of two-level preconditioner

Our choice = The two-level hybrid Schwarz preconditioner [Smith et al., 1996].

Two-level preconditioner
$$\mathcal{P}_{L\&R}$$

 $\mathcal{P}_L := \left[\mathbb{I} - \left(ZE_L^{-1}Z^T\right)M^{-1}A + \left(ZE_L^{-1}Z^T\right)\right]$
 $\mathcal{P}_R := \left[\mathbb{I} - \left(ZE_R^{-1}Z^T\right)AM^{-1} + \left(ZE_R^{-1}Z^T\right)\right]$

$$M^{-1} := \begin{bmatrix} A_{D_{\Omega_1}}^{-1} & 0 & 0 \\ 0 & A_{D_{\Omega_2}}^{-1} & 0 \\ 0 & 0 & A_{D_{\Omega_3}}^{-1} \end{bmatrix}$$

Left preconditioner

$$\mathcal{P}_L M^{-1} A \mathbf{u} = \mathcal{P}_L M^{-1} \mathbf{b}$$

$$E_L := Z^T M^{-1} A Z$$
$$E_R := Z^T A M^{-1} Z$$

Right preconditioner

$$AM^{-1}\mathcal{P}_R\overline{\mathbf{u}} = \mathbf{b}$$

$$\mathbf{u} = M^{-1}\mathcal{P}_R\overline{\mathbf{u}}$$

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New Methods and Techniques Conclusion and Prospects

Academic Problem - 3D Laplace



- all experiments performed on IFP cluster
 - 114 nodes equipped with 4 processes AMD Barcelona 2.3 Ghz (quad-core socket)
 - interconnected by Infiniband switched fabric (type of network topology)
- max number of available process 256
 - thus only in two first variants we dedicated one part per one process

New Methods and Techniques Conclusion and Prospects

What we have measured ?



nitor	number of iterations
mer	number of iterations
κ_{\approx}	roughly estimated condition number given as $\kappa_{pprox} = \lambda_{max}/\lambda_{min}$ where $\lambda_{\{min,max\}}$
	are the approximated, extreme eigenvalues of $(\widetilde{M}^{-1}\widetilde{A})$
nV	number of approximated eigenvectors used in construction of coarse space
$ r_{sol} $	standard norm of final residual i.e., $ r_{sol} = Au_{sol} - b _2/ b _2$
	time of "construction" coarse space operator
Co[s]	time of construction coarse space operator

- Inf[s] time of inflation process for each level
- **LU**[s] time of LU factorisation of endomorphic Partial Operators in DDMOperator
- $\mathbf{sol}[s]$ time of iterative process (in case of varian with two-level preconditioner \mathbf{sol} consist also LU factorisation time of coarse operator)

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New Methods and Techniques

Conclusion and Prospects

Academic Problem - 3D Laplace (SCALABILITY)



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New Methods and Techniques

Conclusion and Prospects

Academic Problem - 3D Laplace (SCALABILITY)



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New Methods and Techniques

ues Conclusion and Prospects

Academic Problem - 3D Laplace (TIME COST)



expvar	niter	κ_{\approx}	nV	$ r_{sol} $	CS [s]	inf[s]	LU[s]	sol[s]
+I(0)	169	15158.70		9.78e - 07			2.04	17.44
+I(1)	101	4818.07		1.68e - 09		1.29	3.56	10.30
D+I(1)	14	5.82	13	2.18e - 06	2.12			5.17
+I(2)	77	2715.89		2.12e - 09		1.29+1.89	7.40	12.63
D+I(2)	12	2.30	10	9.43e - 07	2.20			5.81
+I(3)	64	1820.48		2.64e - 09		1.27+1.87+2.74	13.81	14.57
D+I(3)	13	2.18	7	1.09e - 08	2.00			6.79

	expvar	niter	κ_{\approx}	nV	r _{sol}	CS[8]	int[s]	LU[8]	sol[8]
	+I(0)	115	3694.10		8.31e - 07			2.06	8.84
	+I(1)	69	1174.49		1.92e - 10		1.18	4.39	8.35
D.	+I(1)	15	3.61	10	2.55e - 09	1.18			3.36
	+I(2)	53	662.34		3.09e - 09		1.16+1.73	6.35	6.37
D	+I(2)	15	2.78	5	1.07e - 09	0.76			4.41
	+I(3)	44	444.15		2.59e - 09		1.19+1.76+2.60	14.59	8.03
D.	+I(3)	13	2.37	5	5.46e - 09	1.66			4.91



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New Methods and Techniques

Conclusion and Prospects

100 120

Academic Problem - 3D Laplace (TIME COST)



20

190

170

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New Methods and Techniques Conclusion and Prospects

Real Test Case - SPE10 Benchmark

[from SPE10 description] .. the aim of the SPE10 is to simulate porous media flow in a highly heterogeneous black oil reservoir that is described by a fine-scale 1 million cell geological model.

Matrix spe10_p_only.mtx

nparts	nrows	nnz
256	1,094,421	7,515,591



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New Methods and Techniques

Conclusion and Prospects

IFP Matrices Collection (spe10)



expvar	niter	κ_{\approx}	nV	$ r_{sol} $	CS[s]	inf[s]	LU[s]	sol[s]
+I(0)	700	83147.80		6.40e - 05			1.36	93.34
+I(1)	386	15169.30		3.32e - 08		1.09	2.24	42.14
D+I(1)	80	185.10	10F	1.83e - 09	1.30			22.43
+I(2)	264	7825.55		3.84e - 08		1.09 + 1.54	3.38	22.76
D+I(2)	62	97.08	10F	1.13e - 08	1.48			14.39
+I(3)	211	5055.91		5.02e - 09		1.09 + 1.54 + 2.20	5.06	17.32
D+I(3)	47	50.12	10F	2.22e - 09	1.61			14.22

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New Methods and Techniques Conclusion and Prospects

IFP Matrices Collection (spe10)



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IFP Matrices Collection (ALL)













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New Methods and Techniques Conclusion and Prospects

Black Oil Simulation

Partitioning and data dystribution (mat1)	Ī
LU Factorization of suboperators (mat1)	
SOLVE (mat1) GMRES + Modified Schwarz Method	
Extracting Approximated Eigen Vectors	
Building Coarse Space	
Building Coarse Space Partitioning and data dystribution (mat2)	
Building Coarse Space Partitioning and data dystribution (mat2) LU Factorization of sub-operators (mat2)	

Matrix BO_60x60x32_matX.mtx

mat_name	nparts	nrows	nnz
BO_60x60x32_mat1.mtx	80	115,200	791,520
BO_60x60x32_mat2.mtx	80	115,200	791,572
BO_60x60x32_mat3.mtx	80	115,200	791,598
BO_60x60x32_mat4.mtx	80	115,200	791,500
BO_60x60x32_mat5.mtx	80	115,200	791,512

Matrix BO_120x120x64_matX.mtx

mat_name	nparts	nrows	nnz
BO_120x120x64_mat1.mtx	160	921,600	6,391,680
B0_120x120x64_mat2.mtx	160	921,600	6,391,680
BO_120x120x64_mat3.mtx	160	921,600	6,391,680
B0_120x120x64_mat4.mtx	160	921,600	6,390,986
B0_120x120x64_mat5.mtx	160	921,600	6,387,222

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Black Oil Simulation







		$\sum [s]$			
ASM+I(1)	5×7.58	37.90			
ASM+I(1)+D	$1{\times}7.58 + 1.27 + 4{\times}3.67$	23.53			
			<u> </u>	10	

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Conclusion and Prospects

Black Oil Simulation - Reduced Formula

 $\widetilde{\mathcal{P}}_R := \left[\mathbb{I} - (ZE_R^{-1}Z^T)AM^{-1} + (ZE_R^{-1}Z^T) \right]$





- We have considered the extended and the original linear system arising from the domain decomposition method with overlapping.
- We applied the two-level preconditioner using Schwarz algorithm and the coarse grid correction
- 3 The coarse grid space is based on the approximated (sub-domain wise split) eigenvectors
 - its size can be adapted to the difficulty of the problem
- ④ All presented methods are as algebraic as possible which paves the way to extension to systems of equations e.g. multiphase flows
- Proposed two-level preconditioner is scalable and can be very robust in respect to number of iteration
- Both methods are adaptive and can be used during first solve that is even the first solve is not completed
- 7 All methods work for arbitrary decomposition
 - which quality we can improve using weighted graph partitioning

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New Methods and Techniques Conclusion and Prospects



Dziekuje za wasza uwage!



Merci de votre attention!



Thank you for your attention!

Bibliography I

Buluc, A., Fineman, J. T., Frigo, M., Gilbert, J. R., and Leiserson, C. E. (2009).

Parallel sparse matrix-vector and matrix-transpose-vector multiplication using compressed sparse blocks.

In SPAA '09: Proceedings of the twenty-first annual symposium on Parallelism in algorithms and architectures, pages 233-244, New York, NY, USA, ACM.



Lions, P.-L. (1990).

On the Schwarz alternating method. III: a variant for nonoverlapping subdomains.

In Chan, T. F., Glowinski, R., Périaux, J., and Widlund, O., editors, Third International Symposium on Domain Decomposition Methods for Partial Differential Equations held in Houston, Texas, March 20-22, 1989, Philadelphia, PA. SIAM.

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Bibliography II

Magoulès, F., Roux, F. X., and Series, L. (2006). Algebraic approximation of dirichlet-to-neumann maps for equations of linear elasticity.

Comp. Meth. Appl. Mech. Engrg., 195:3742–3759.

- Nataf, F., Rogier, F., and de Sturler, E. (1994). Optimal interface conditions for domain decomposition methods. Technical Report 301, CMAP (Ecole Polytechnique).
- Nicolaides, R. A. (1987).

Deflation of conjugate gradients with applications to boundary value problems.

SIAM J. Matrix Anal. Appl., 24:355-365.



Schwarz, H. A. (1870).

Über einen Grenzübergang durch alternierendes Verfahren. Vierteljahrsschrift der Naturforschenden Gesellschaft in Zürich, 15:272-286.

Bibliography III

Smith, B. F., Bjørstad, P. E., and Gropp, W. (1996). Domain Decomposition: Parallel Multilevel Methods for Elliptic Partial Differential Equations. Cambridge University Press.



Stüben, K. (2001).

A review of algebraic multigrid.

Journal of Computational and Applied Mathematics, 128:281–309.



Tang, J. M., Nabben, R., Vuik, C., and Erlangga, Y. A. (2009). Comparison of two-level preconditioners derived from deflation, domain decomposition and multigrid methods.

J. Sci. Comput., 39:340-370.

Additional Numerical Experiments

IFP Matrices Collection (spe10 - system of equations)



expvar	niter	$ r_{sol} $	$\inf[s]$	LU[s]	sol[s]
+I(0)	663	1.43e - 06		≈ 4	343.13
+I(1)	361	2.12e - 09	4.36	≈ 6	70.76
+I(2)	252	3.81e - 08	4.37 + 7.23	≈ 13	70.88
+I(3)	183	2.03e - 08	4.52 + 7.42 + 11.00	≈ 24	78.14

Sparse Patch Method

Adaptive Solver



$$\mathcal{K}_{m}^{\mathrm{ASM}}\left(\mathrm{AM}^{-1},\mathbf{r}_{0}\right) := \mathbf{u}_{0} + \operatorname{SPAN}\left\{\mathbf{r}_{0},(\mathrm{AM}^{-1})^{m-1}\mathbf{r}_{0}\right\}$$
$$\mathcal{K}_{m}^{2l\nu l}\left(\mathrm{AM}^{-1}\mathscr{P}_{\mathrm{R}},\mathbf{r}_{0}\right) := \mathbf{u}_{0} + \operatorname{SPAN}\left\{\mathbf{r}_{0},(\mathrm{AM}^{-1}\mathscr{P}_{\mathrm{R}})^{m-1}\mathbf{r}_{0}\right\}$$

Adaptive Solver - Stop after XX


Adaptive Solver - Stop after 10



Adaptive Solver - Stop after 20



Adaptive Solver - Stop after (40 and 50)



Adaptive Solver vs Time of Computation



expvar	niter	κ_{\approx}	nV nV	$ r_{sol} $	$\ $	$\mathbf{CS}[s]$	$\inf[s]$	LU[s]	$\mathbf{sol}[s]$
+I(1)	101	4818.07		1.68e - 09			1.29	3.56	10.30
S10	10 + 85	2427.91	2	2.34e - 09	ľ	0.25	1.38	4.21	3.43 + 12.15
S20	20 + 56	648.32	3	1.22e - 0.9	1	0.37	1.31	4.17	3.52 + 11.77
S40	40 + 23	7.68	6	9.53e - 10	ľ	1.15	1.32	5.47	3.73 + 7.70
S50	50 + 18	4.12	8	2.69e - 10		1.01	1.29	3.76	3.91 + 3.82

Adaptive Solver vs Time of Computation



Improved Diagonal Approximation (EDOIC)

Improved Diagonal Approximation (EDOIC)

Let $\beta_{\widetilde{1}_c\widetilde{1}_c}$ be a symmetric sparse operator which satisfies

$$\beta_{\widetilde{1}_{c}\widetilde{1}_{c}}A_{\widetilde{1}_{c}\widetilde{1}_{c}}V_{\widetilde{1}_{c}} = V_{\widetilde{1}_{c}}, \quad \text{or equivalently} \quad -\beta_{\widetilde{1}_{c}\widetilde{1}_{c}}A_{\widetilde{1}_{c}\widetilde{\Gamma}_{1}}V_{\widetilde{\Gamma}_{1}} = V_{\widetilde{1}_{c}}.$$

The optimal interface conditions operator $S^{opt}_{\widetilde{\Gamma}_1\widetilde{\Gamma}_1}$ is approximated by

$$S^{opt}_{\widetilde{\Gamma}_{1}\widetilde{\Gamma}_{1}} \approx S^{edoic}_{\widetilde{\Gamma}_{1}\widetilde{\Gamma}_{1}} := -A_{\widetilde{\Gamma}_{1}\widetilde{1}_{c}} \left(2\beta_{\widetilde{1}_{c}\widetilde{1}_{c}} - \beta_{\widetilde{1}_{c}\widetilde{1}_{c}}A_{\widetilde{1}_{c}\widetilde{1}_{c}}\beta_{\widetilde{1}_{c}\widetilde{1}_{c}}\right) A_{\widetilde{1}_{c}\widetilde{\Gamma}_{1}}$$

The idea of this improvement originates from the following calculations: $\|(\mathcal{B}\mathcal{A}-I)\| \leq \epsilon < 1$ leads to $\|(\mathcal{B}\mathcal{A}-I)^2\| \leq \epsilon^2 < \epsilon$. Then, remarking that $(\mathcal{B}\mathcal{A}-I)^2 = \mathcal{B}\mathcal{A}\mathcal{B}\mathcal{A} - 2\mathcal{B}\mathcal{A} + I = I - (2\mathcal{B}-\mathcal{B}\mathcal{A}\mathcal{B})\mathcal{A}$, one concludes that $\mathcal{C} = 2\mathcal{B} - \mathcal{B}\mathcal{A}\mathcal{B}$ is better approximation of \mathcal{A}^{-1} than \mathcal{B} since $\|\mathcal{C}-I\| \leq \epsilon^2 < \epsilon$.

Sparse Patch Method

Sparse Patch Method



See [Magoulès et al., 2006] for more informations.