Optimized Schwarz Methods

Frédéric Nataf *

February 12, 2009

*Laboratoire J.L. Lions, CNRS UMR7598, Paris, France. nataf@ann.jussieu.fr www.ann.jussieu.fr/~nataf

Outline

- 1. Motivation
- 2. Schwarz method (1860)
- 3. Two families of methods

Schur Complement type methods (Neumann-Neumann, FETI, BDDC, FETI-DP, ...

Optimized Interface Conditions

Coarse grid issues

- 4. Non conforming methods in space (and time)
- 5. Laser-Plasma Interaction via HPC

Why Domain Decomposition Methods ?

- In some situations, the decomposition is natural
 - Moving domains (rotor and stator in an electric motor)
 - Strongly heterogeneous media : Sliding blocks along faults in subsurface modeling
 - Different physics in different subdomains
 - ⇒ Tools for handling non conforming mesh are needed "Domain connection" would be more appropriate
- Parallel processing is the only way to have faster codes New generation processors are parallel: dual, quadri core,
- Large scale computations \implies need for an "artificial" decomposition

Memory requirements

Direct solvers are too costly and iterative solvers are not robust enough \implies New iterative/direct solvers are welcome : these are domain decomposition methods

Linear Algebra from the End User point of view

Direct Solvers	DDM	Krylov
Cons: Memory	Pro: Flexible Compromise	Pros: Memory
Difficult to parallelize	Parallel computer	Easy to parallelize
Pros: Robustness		Cons: Robustness
solve(MAT,RHS,SOL)	Few black box routines	solve(MAT,RHS,SOL)
	Partial implementation	
	of efficient DDM	

Multigrid methods: very efficient but may lack robustness, not always applicable (Helmholtz type problems, complex systems) and difficult to parallelize.

The First Domain Decomposition Method The original Schwarz Method (H.A. Schwarz, 1870) Ω_2 Ω₁ $-\Delta(u) = f$ in Ω

u = 0 on $\partial \Omega$.

Schwarz Method : $(u_1^n, u_2^n) \rightarrow (u_1^{n+1}, u_2^{n+1})$ with

$$-\Delta(u_1^{n+1}) = f \quad \text{in } \Omega_1 \qquad -\Delta(u_2^{n+1}) = f \quad \text{in } \Omega_2$$
$$u_1^{n+1} = 0 \text{ on } \partial\Omega_1 \cap \partial\Omega \qquad u_2^{n+1} = 0 \text{ on } \partial\Omega_2 \cap \partial\Omega$$
$$u_1^{n+1} = u_2^n \quad \text{on } \partial\Omega_1 \cap \overline{\Omega_2}. \qquad u_2^{n+1} = u_1^{n+1} \quad \text{on } \partial\Omega_2 \cap \overline{\Omega_1}$$

Parallel algorithm, converges but very slowly, overlapping subdomains only. Improvement will come from: 1) introducing Krylov methods, 2) Neumann or 3) more general boundary conditions and 4) coarse grid corrections

Introducing Krylov Methods

Fixed point methods are intrinsically slower than Krylov methods Solve

$$Ax = b$$

by a fixed point method with a linear operator B easy to invert:

$$Bx^{n+1} = Bx^n + (b - Ax^n)$$

Let $r_0 := b - Ax^0$, we have:

$$x^{n} = \sum_{i=0}^{n} (I_{d} - B^{-1}A)^{i} B^{-1}r_{0} + x^{0}$$

A preconditioned Krylov solve will generate an optimal x_K^n in

 $\mathcal{K}^{n}(B^{-1}A, B^{-1}r_{0}) := x_{0} + Span\{B^{-1}r_{0}, B^{-1}AB^{-1}r_{0}, \dots, (B^{-1}A)^{n}B^{-1}r_{0}\}$

and since $x^n \in \mathcal{K}^n(B^{-1}A, B^{-1}r_0)$ as well but with "frozen" coefficients $\Rightarrow x_n$ is less optimal (actually much much less) than x_K^n

Jacobi and Schwarz (I): Algebraic point of view

The set of indices is partitioned into two sets \mathcal{N}_1 and \mathcal{N}_2 :

$$\left(\begin{array}{cc}A_{11} & A_{12}\\A_{21} & A_{22}\end{array}\right)\left(\begin{array}{c}x_1\\x_2\end{array}\right) = \left(\begin{array}{c}b_1\\b_2\end{array}\right)$$

The block-Jacobi algorithm reads:

$$\begin{pmatrix} A_{11} & 0 \\ 0 & A_{22} \end{pmatrix} \begin{pmatrix} x_1^{k+1} \\ x_2^{k+1} \end{pmatrix} = -\begin{pmatrix} 0 & A_{12} \\ A_{21} & 0 \end{pmatrix} \begin{pmatrix} x_1^k \\ x_2^k \end{pmatrix} + \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$$

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

$$\begin{array}{c}
1 \\
2 \\
\hline
1 \\
\overline{1} \\
\overline{2}
\end{array}$$

Figure 1: Domain decomposition with minimal overlap

Jacobi and Schwarz (II): Larger overlap

Let δ be a non negative integer



Figure 2: Domain decomposition with overlap



Figure 3: Matrix decomposition Without or with overlap

Krylov - Schwarz

Schwarz method is a fixed point method of Jacobi style

$$T: \ (x^k, b) \longmapsto x^{k+1}$$

which solves the linear system:

$$(I_d - T(\cdot, 0))(x) = T(0, b)$$

Use instead Krylov type method : CG, GMRES, BICGSTAB, ... Gain :

- Iteration count : $\kappa \longrightarrow \sqrt{\kappa}$
- Robustness

In practice, you get a factor three or more.

For some time-dependent problems discretized with a small time step, results are satisfactory. Otherwise, the method is slow. Improvement will come from the introduction of Neumann or more general BCs

First family of modern methods : Substructuring formulation

We want to solve

$$\mathcal{L}(u) := -\Delta(u) = f \text{ in } \Omega$$

 $u = 0 \text{ on } \partial \Omega.$

The domain is decomposed into two non overlapping subdomains. Let u_1 and u_2 be the solutions in the subdomains and





First family of modern methods : Substructuring formulation

Consider a non overlapping decomposition of the domain Ω into Ω_1 and Ω_2 and Dirichlet BVP in each subdomain with $u|_{\Gamma}$ as a Dirichlet data

$$-\Delta(u_i) = f \quad \text{in } \Omega_i,$$
$$u_i = u|_{\Gamma} \quad \text{on } \Gamma, \quad u_i = 0 \quad \text{sur } \partial \Omega_i \backslash \Gamma.$$

The jump of the normal derivative across the interface is a function of f and $u|_{\Gamma}$

$$\mathcal{S}(f, u|_{\Gamma}) = \frac{1}{2} \left(\frac{\partial u_1}{\partial n_1} + \frac{\partial u_2}{\partial n_2} \right)|_{\Gamma}$$

The substructured interface problem reads : Find $u|_{\Gamma}$ s.t.

$$\mathcal{S}(0, u|_{\Gamma}) = -\mathcal{S}(f, 0)$$

The corresponding discrtized problem is solved by a Krylov type method such as CG, GMRES, BICGSTAB, QMR, ...

- Gain: if $\kappa(-\Delta_h) = O(1/h^2)$, then $\kappa(\mathcal{S}_h) = O(1/h)$.
- Extension : Find a good preconditioner \mathcal{T}_h s.t. $\kappa(\mathcal{T}_h S_h) \simeq O(1).$

Neumann-Neumann alg. for the Laplace equation

(Bourgat, Glowinski, Le Tallec and Vidrascu, 1989) The idea is to approximate the inverse of $\mathcal{S}(0, .)$ by \mathcal{T} :

$$\mathcal{T}: H^{-\frac{1}{2}}(\Gamma) \to H^{\frac{1}{2}}_{00}(\Gamma)$$
$$\mathcal{T}(g) = \frac{1}{2} (v_1 + v_2) |_{\Gamma}.$$

where

$$\mathcal{L}v_i = 0 \quad \text{in } \Omega_i,$$
$$\frac{\partial v_i}{\partial n_i} = g \quad \text{sur } \Gamma$$

Optimality

The preconditioned operator $\mathcal{TS}(0,.)$ is a continuous operator from $H_{00}^{\frac{1}{2}} \to H_{00}^{\frac{1}{2}}$. After discretization and with an adequate coarse grid, the condition number is $\log(h)$.

Complexity

difficult to extend to arbitrary systems of PDEs, ill-posed subproblems, needs matrix before assembly, ...

FETI method for the Laplace problem

We first consider Neumann problems in each subdomain

$$\mathcal{L}(u_i) = f \quad \text{in } \Omega_i,$$

$$\frac{\partial u_i}{\partial n_i} = (-1)^{i+1} \lambda|_{\Gamma} \quad \text{on } \Gamma$$

$$u_i = 0 \quad \text{sur } \partial \Omega_i \backslash \Gamma.$$

We consider the Neuman to Dirichlet (NtD) map

$$\mathcal{T}_{feti}: L^2(\Omega) \times H^{-\frac{1}{2}}(\Gamma) \to H^{\frac{1}{2}}_{00}(\Gamma)$$
$$\mathcal{T}_{feti}(f, \lambda|_{\Gamma}) = \frac{1}{2} \left(u_1 - u_2 \right)|_{\Gamma}$$

The substructured problem reads:

$$\mathcal{T}_{feti}(0, \boldsymbol{\lambda}|_{\Gamma}) = -\mathcal{T}_{feti}(f, 0)$$

The corresponding discretized problem is solved by a Krylov type method preconditioned by $\mathcal{S}(.,0)$. The preconditioner consists in solving Dirichlet problems. (Farhat, Roux, Widlund, ...)

Another possible Improvement: other interface conditions

(P.L. Lions, 1988)

$$-\Delta(u_1^{n+1}) = f \quad \text{in } \Omega_1,$$

$$u_1^{n+1} = 0 \quad \text{on } \partial\Omega_1 \cap \partial\Omega,$$

$$(\frac{\partial}{\partial n_1} + \alpha)(u_1^{n+1}) = (-\frac{\partial}{\partial n_2} + \alpha)(u_2^n) \quad \text{on } \partial\Omega_1 \cap \overline{\Omega_2},$$

 $(n_1 \text{ and } n_2 \text{ are the outward normal on the boundary of the subdomains})$

$$-\Delta(u_2^{n+1}) = f \quad \text{in } \Omega_2,$$

$$u_2^{n+1} = 0 \quad \text{on } \partial\Omega_2 \cap \partial\Omega$$

$$(\frac{\partial}{\partial n_2} + \alpha)(u_2^{n+1}) = (-\frac{\partial}{\partial n_1} + \alpha)(u_1^n) \quad \text{on } \partial\Omega_2 \cap \overline{\Omega_1}.$$

with $\alpha > 0$. Overlap is not necessary for convergence. Extended to the Helmholtz equation (B. Desprès, 1991) a.k.a FETI 2 LM (Two-Lagrange Multiplier) Method, 1998.

- Gain: Much faster convergence, no need for overlaps
- Extensions:

Find even better interface conditions (Optimized Interface Conditions)

introduce Krylov type methods in place of the above fixed point algorithm (already seen).

Optimized Schwarz Methods

- 1. Optimal Interface Conditions
- 2. Optimized Interface Conditions
- 3. Application to the Helmholtz equation
- 4. Optimized IC Discontinuous coefficients equations
- 5. Conclusion

(Recall) One possible Improvement: other interface conditions

(P.L. Lions, 1988)

$$-\Delta(u_1^{n+1}) = f \quad \text{in } \Omega_1,$$

$$u_1^{n+1} = 0 \quad \text{on } \partial\Omega_1 \cap \partial\Omega,$$

$$(\frac{\partial}{\partial n_1} + \alpha)(u_1^{n+1}) = (-\frac{\partial}{\partial n_2} + \alpha)(u_2^n) \quad \text{on } \partial\Omega_1 \cap \overline{\Omega_2},$$

 $(n_1 \text{ and } n_2 \text{ are the outward normal on the boundary of the subdomains})$

$$-\Delta(u_2^{n+1}) = f \quad \text{in } \Omega_2,$$

$$u_2^{n+1} = 0 \quad \text{on } \partial\Omega_2 \cap \partial\Omega$$

$$(\frac{\partial}{\partial n_2} + \alpha)(u_2^{n+1}) = (-\frac{\partial}{\partial n_1} + \alpha)(u_1^n) \quad \text{on } \partial\Omega_2 \cap \overline{\Omega_1}.$$

with $\alpha > 0$. Overlap is not necessary for convergence. Extended to the Helmholtz equation (B. Desprès, 1991) a.k.a FETI 2 LM (Two-Lagrange Multiplier) Method, 1998.

Convergence with second order interface conditions

$$\left(\frac{\partial}{\partial n_i} + \alpha - \frac{\partial}{\partial \tau}\gamma \frac{\partial}{\partial \tau}\right)$$

Proof of convergence valid for a problem discretized by a finite volume scheme. At the continuous level we consider the following problem.

$$\eta(\mathbf{x})u - div(\kappa(\mathbf{x})\nabla u) = f \quad \text{in } \Omega,$$
$$u = 0 \quad \text{on } \partial\Omega,$$

with $\eta(\mathbf{x}), \kappa(\mathbf{x}) > C > 0$. The domain is decomposed into N subdomains $(\Omega_i)_{1 \le i \le N}$ without overlap. Let Γ_{ij} denote the interface $\Gamma_{ij} = \partial \Omega_i \cap \partial \Omega_j$.

Convergence

The interface condition is

$$\kappa(\mathbf{x})\frac{\partial u_i^{n+1}}{\partial n_i} + \alpha_{ij}(\mathbf{x})u_i^{n+1} - \frac{\partial}{\partial \tau_i}(\gamma_{ij}(\mathbf{x})\frac{\partial u_i^{n+1}}{\partial \tau_i})$$
$$= -\kappa(\mathbf{x})\frac{\partial u_j^n}{\partial n_j} + \alpha_{ij}(\mathbf{x})u_j^n - \frac{\partial}{\partial \tau_j}(\gamma_{ij}(\mathbf{x})\frac{\partial u_j^n}{\partial \tau_j}) \text{ on } \Gamma_{ij}.$$

with

$$\alpha_{ij}(\mathbf{x}) = \alpha_{ji}(\mathbf{x}) \ge \alpha_0 > 0,$$

$$\gamma(\mathbf{x})_{ij} = \gamma(\mathbf{x})_{ji} \ge 0 \text{ et } \gamma_{ij}(\mathbf{x}) = 0 \text{ sur } \partial \Gamma_{ij}$$

Let us denote

$$\Lambda_{ij} = \alpha_{ij}(\mathbf{x}) - \frac{\partial}{\partial \tau_i} (\gamma_{ij}(\mathbf{x}) \frac{\partial}{\partial \tau_i}), \quad \mathbf{x} \in \Gamma_{ij}.$$

Lemma 1 The algorithm converges in H^1 (discrete norm).

The convergence rate is very sensitive to α and γ , how to choose them?

(Hagstrom, 1988)

Constant coefficient Advection-Diffusion equation on a domain decomposed into two subdomains.

$$(\vec{a}\nabla - \nu\Delta)(u_1^{n+1}) = f \quad \text{in } \Omega_1,$$

$$u_1^{n+1} = 0 \quad \text{on } \partial\Omega_1 \cap \partial\Omega,$$

$$(\frac{\partial}{\partial n_1} + \mathcal{B}_1)(u_1^{n+1}) = (-\frac{\partial}{\partial n_2} + \mathcal{B}_1)(u_2^n) \quad \text{on } \partial\Omega_1 \cap \overline{\Omega_2},$$

$$(\vec{a}\nabla - \nu\Delta)(u_2^{n+1}) = f \quad \text{in } \Omega_2,$$

$$u_2^{n+1} = 0 \quad \text{on } \partial\Omega_2 \cap \partial\Omega$$

$$(\frac{\partial}{\partial n_2} + \mathcal{B}_2)(u_2^{n+1}) = (-\frac{\partial}{\partial n_1} + \mathcal{B}_2)(u_1^n) \quad \text{on } \partial\Omega_2 \cap \overline{\Omega_1}.$$

where \mathcal{B}_i , i = 1, 2 are defined via a Fourier transform along the interface

Convergence in two iterations

Let us consider the problem

$$\mathcal{L}_{i}(P_{i}) = f \quad \text{in } \Omega_{i}, \quad i = 1, 2$$
$$P_{1} = P_{2} \quad \text{on } \Gamma_{12},$$
$$\kappa_{1} \frac{\partial P_{1}}{\partial n_{1}} + \kappa_{2} \frac{\partial P_{2}}{\partial n_{2}} = 0 \quad \text{on } \Gamma_{12}.$$

where

$$\mathcal{L}_i = \eta_i - div(\kappa_i \nabla)$$

Could be as well Fluid/Structure interaction or Plate/beam coupling.

Let

$$u_i = \kappa_i \nabla P_i$$

Let us consider a Schwarz type method:

$$\mathcal{L}_{1}(P_{1}^{n+1}) = f \quad \text{in } \Omega_{1} \qquad \qquad \mathcal{L}_{2}(P_{2}^{n+1}) = f \quad \text{in } \Omega_{2}$$

$$P_{1}^{n+1} = 0 \text{ on } \partial\Omega_{1} \cap \partial\Omega \qquad \qquad P_{2}^{n+1} = 0 \text{ on } \partial\Omega_{2} \cap \partial\Omega$$

$$u_{1}^{n+1}.\vec{n}_{1} + \mathcal{B}_{1}(P_{1}^{n+1}) \qquad \qquad u_{2}^{n+1}.\vec{n}_{2} + \mathcal{B}_{2}(P_{2}^{n+1})$$

$$= -u_{2}^{n}.\vec{n}_{2} + \mathcal{B}_{1}(P_{2}^{n}) \quad \text{on } \Gamma_{1} \qquad \qquad = -u_{1}^{n}.\vec{n}_{1} + \mathcal{B}_{2}(P_{1}^{n}) \quad \text{on } \Gamma_{2}$$

We take

$$\mathcal{B}_1 = DtN_2.$$

and have convergence in two iterations.

We introduce the DtN (Dirichlet to Neumann) map (a.k.a. Steklov-Poincaré):

Let
$$P_0: \Gamma_{12} \to \mathbb{R}$$
 (1)
 $DtN_2(P_0) \equiv \kappa_2 \frac{\partial}{\partial n_2} (P)_{|\Gamma_{12}}$

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

$$\mathcal{L}(P) = 0 \text{ in } \Omega_2$$
$$P = 0 \text{ on } \partial \Omega_2 \backslash \Gamma_i$$
$$P = P_0 \text{ on } \Gamma_{12}.$$

We take

$$\mathcal{B}_1 = DtN_2.$$

(Rogier, de Sturler and N., 1993)

The result can be generalized to variable coefficients operators and a decomposition of the domain Ω in more than two subdomains. For the following geometries,



one can define interface conditions such as to have convergence in a number of iterations equals to the number of subdomains. For arbitrary decompositions, negative conjectures have been formulated (F. Nier, *Séminaire X-EDP*, 1998).

Conditions d'interface optimisées analytiques dans le cas scalaire

The Steklov-Poincaré DtN is not a partial differential operator. It is

1. non local

2. its explicit form is not known in the general case

It is approximated by a partial differential operator

$$DtN \simeq \alpha_{opt} - \frac{\partial}{\partial \tau} (\gamma_{opt} \frac{\partial}{\partial \tau})$$

trying to minimize the convergence rate of the algorithm. We speak of optimized of order 2 (opt2) interface conditions If we take $\gamma = 0$ and optimize only with respect to α , we speak of optimized of order 0 (opt0)

A model problem

$$\mathcal{L}(u) := \eta u - \Delta u = f \text{ in } \mathbb{R}^2, \quad \eta > 0$$

The plane \mathbb{R}^2 is divided into two half-planes with an overlap of size $\delta \geq 0$ and the algorithm writes:

$$\mathcal{L}(u_1^{n+1}) = f \quad \text{in } \Omega_1 :=] - \infty, \delta[\times \mathbb{R},$$

$$(\frac{\partial}{\partial n_1} + \alpha)(u_1^{n+1}) = (-\frac{\partial}{\partial n_2} + \alpha)(u_2^n) \quad \text{at } x = \delta$$

$$\mathcal{L}(u_2^{n+1}) = f \quad \text{in } \Omega_2 :=]0, \infty[\times \mathbb{R},$$

$$(\frac{\partial}{\partial n_2} + \alpha)(u_2^{n+1}) = (-\frac{\partial}{\partial n_1} + \alpha)(u_1^n) \quad \text{at } x = 0$$

A Fourier analysis leads to the following convergence rate (k is the dual variable):

$$\rho(k;\delta,\alpha) = \left| \frac{\sqrt{\eta + k^2} - \alpha}{\sqrt{\eta + k^2} + \alpha} \right| e^{-\sqrt{\eta + k^2}} \delta$$

Optimizing the interface condition

In the physical space:

$$\rho(\delta, \alpha) = \max_{|k| \le 1/h} \left| \frac{\sqrt{\eta + k^2} - \alpha}{\sqrt{\eta + k^2} + \alpha} \right| \, e^{-\sqrt{\eta + k^2}} \delta$$

When there is no overlap $(\delta = 0)$:

- if α is h independent, then $\rho \simeq 1 C^t h$
- if α varies like 1/h, then $\rho \simeq 1 C^t h$
- if α solves the min-max problem:

$$\rho(\alpha_{opt}) := \min_{\alpha > 0} \max_{|k| \le 1/h} \rho(k; 0, \alpha)$$

then α_{opt} varies like $1/\sqrt{h}$ and $\rho_{opt} \simeq 1 - C^t \sqrt{h}$ With overlap

- Classical Schwarz: $\alpha = \infty$, $\rho_{Scwharz} > \rho_{\alpha}$, $\forall \alpha$
- Optimization for small h with $\delta = C h$, (Gander, SISC, 2006)

$1/\Delta y$	10	20	40	80
$lpha_{ m opt}^{ m sc}$	6	7	10	16
$\alpha = 1$	27	51	104	231

Table 1: Number of iterations for different values of the mesh size and two possible choices for α , no overlap

Application: the Helmholtz Equation

Joint work with M. Gander and F. Magoulès SIAM J. Sci. Comp., 2002.

We want to solve

$$-\omega^2 u - \Delta u = f \quad \text{in } \Omega$$
$$u = 0 \quad \text{on } \partial \Omega.$$

The relaxation algorithm is : $(u_1^p, u_2^p) \to (u_1^{p+1}, u_2^{p+1})$ with $(i \neq j, i = 1, 2)$

$$(-\omega^2 - \Delta)(u_i^{p+1}) = f \quad \text{in } \Omega_i$$
$$(\frac{\partial}{\partial n_i} + \mathcal{S})(u_i^{p+1}) = (-\frac{\partial}{\partial n_j} + \mathcal{S})(u_j^p) \quad \text{on } \Gamma_{ij}.$$
$$u_i^{p+1} = 0 \text{ on } \partial \Omega_i \cap \partial \Omega$$

The operator \mathcal{S} has the form

$$\mathcal{S} = \alpha - \gamma \frac{\partial^2}{\partial \tau^2} \qquad \boldsymbol{\alpha}, \boldsymbol{\gamma} \in \mathbb{C}$$

Application: the Helmholtz Equation

By choosing carefully the coefficients α and γ , it is possible to optimize the convergence rate of the iterative method which in the Fourier space is given by

$$\rho(k;\alpha,\gamma) \equiv \begin{cases} \left| \frac{I\sqrt{\omega^2 - k^2} - (\alpha + \gamma k^2)}{I\sqrt{\omega^2 - k^2} + (\alpha + \gamma k^2)} \right| & \text{if } |k| < \omega \quad (I^2 = -1) \\ \\ \left| \frac{\sqrt{k^2 - \omega^2} - (\alpha + \gamma k^2)}{\sqrt{k^2 - \omega^2} + (\alpha + \gamma k^2)} \right| & \text{if } |k| > \omega \end{cases}$$

Finally, we get analytic formulas for α and γ (*h* is the mesh size):

$$\alpha_{opt} = \alpha(\omega, h) \text{ and } \gamma_{opt} = \gamma(\omega, h),$$

Moreover, a Krylov method (GC, GMRES, BICGSTAB, ...) replaces the fixed point algorithm.

The Helmholtz Equation – Numerical Results

Waveguide: Optimized Schwarz method with QMR compared to ABC0 $(\partial_n + I\omega)$ with relaxation on the interface



Discretization of the two-field formulation

A direct discretization would require the computation of the normal derivatives along the interfaces in order to evaluate the right handsides.

In order to avoid this extra task, we introduce two new variables

$$\lambda^1 = -\frac{\partial u_2}{\partial n_2} + \mathcal{S}(u_2) \text{ and } \lambda^2 = -\frac{\partial u_1}{\partial n_1} + \mathcal{S}(u_1).$$

The algorithm reads now

$$-\Delta u_1^{n+1} + \omega^2 u_1^{n+1} = f \text{ in } \Omega_1$$
$$\frac{\partial u_1^{n+1}}{\partial n_1} + \mathcal{S}(u_1^{n+1}) = \lambda^{1n} \text{ on } \Gamma_{12}$$

$$-\Delta u_2^{n+1} + \omega^2 u_2^{n+1} = f \text{ in } \Omega_2$$
$$\frac{\partial u_2^{n+1}}{\partial n_2} + \mathcal{S}(u_2^{n+1}) = \lambda^{2^n} \text{ on } \Gamma_{12}$$

$$\lambda^{1^{n+1}} = -\lambda^{2^n} + (S + S)(u_2^{n+1}(\lambda^{1^p}, f))$$
$$\lambda^{2^{n+1}} = -\lambda^{1^n} + (S + S)(u_1^{n+1}(\lambda^{2^p}, f)).$$

This new formulation paves the way for the replacement of the fixed point algorithm by Krylov type methods (e.g. QMR, ORTHODIR) which are both more efficient and more reliable.

Finite Element Discretization

A finite element discretization leads to the following linear system:

$$\lambda^{1} = -\lambda^{2} + (S+S)B^{2}u^{2}$$
$$\lambda^{2} = -\lambda^{1} + (S+S)B^{1}u^{1}$$
$$\widetilde{K}^{1}u^{1} = f^{1} + B^{1^{T}}\lambda^{1}$$
$$\widetilde{K}^{2}u^{2} = f^{2} + B^{2^{T}}\lambda^{2}$$
(2)

where B^1 (resp. B^2) is the trace operator of domain Ω^1 (resp. Ω^2) on the interface Γ_{12} . Matrix \widetilde{K}^i , i = 1, 2 arises from the discretization of the local Helmholtz subproblems along with the interface condition $\partial_n + \alpha - \gamma \partial_{\tau\tau}$.

$$\widetilde{K}^{i} = K^{i} - \omega^{2} M^{i} + B^{i^{T}} (\alpha M_{\Gamma_{12}} + \gamma K_{\Gamma_{12}}) B^{i}$$
(3)

where K^i is the stiffness matrix, M^i the mass matrix, $M_{\Gamma_{12}}$ is the interface mass matrix and $K_{\Gamma_{12}}$ is the interface stiffness matrix.

More precisely, the interface mass matrix $M_{\Gamma_{12}}$ and the interface stiffness matrix $K_{\Gamma_{12}}$ are defined by

$$[M_{\Gamma_{12}}]_{lm} = \int_{\Gamma_{12}} \phi_l \phi_m d\xi \quad \text{and} \quad [K_{\Gamma_{12}}]_{lm} = \int_{\Gamma_{12}} \nabla_\tau \phi_l \nabla_\tau \phi_m d\xi \quad (4)$$

where ϕ_l et ϕ_m are the basis functions associated to nodes l and mon the interface Γ_{12} and $\nabla_{\tau}\phi$ is the tangential component of $\nabla\phi$ on the interface.

We have

$$S = \alpha M_{\Gamma_{12}} + \gamma K_{\Gamma_{12}}.$$

The substructured linear system of the two-field formulation has the form

$$F\lambda = d \tag{5}$$

where $\lambda = (\lambda^1, \lambda^2)$, F is a matrix and d is the right hand side

$$F = \begin{bmatrix} I & I - (S+S)B^{2}\tilde{K}^{2^{-1}}B^{2^{T}} \\ I - (S+S)B^{1}\tilde{K}^{1^{-1}}B^{1^{T}} & I \end{bmatrix}$$
$$d = \begin{bmatrix} (S+S)B^{1}\tilde{K}^{1^{-1}}f^{1} \\ (S+S)B^{2}\tilde{K}^{2^{-1}}f^{2} \end{bmatrix}$$

The linear system is solved by a Krylov type method, here the ORTHODIR algorithm. The matrix vector product amounts to solving a subproblem in each subdomain and to send interface data between subdomains.

General Interface Conditions for the Helmholtz Equation Numerical Results

Waveguide: Optimized Schwarz method with QMR and ABC0 $(\partial_n + I\omega)$ with relaxation on the interface



General Interface Conditions for the Helmholtz Equation Numerical Results: Acoustic in a Car



Numerical Results: Acoustic in a Car



General Interface Conditions for the Helmholtz Equation Numerical Results

Acoustic in a Car : Iteration Counts for various interface conditions

N_s	ABC 0	ABC 2	Optimized
2	16 it	16 it	9 it
4	50 it	52 it	15 it
8	83 it	93 it	25 it
16	105 it	133 it	34 it

ABC 0: Absorbing Boundary Conditions of Order 0 $(\partial_n + I\omega)$ ABC 2: Absorbing Boundary Conditions of Order 2 $(\partial_n + I\omega - 1/(2I\omega)\partial_{y^2})$ Optimized: Optimized Interface Conditions

Motor compartment



Frequency	Number of sub-domains	Order Zero		Order Two	
		Taylor	Optimized	Taylor	Optimized
600	2	451	205	453	147
600	4	573	287	625	186
600	8	715	355	803	237
800	2	447	221	445	146
800	4	647	323	733	212
800	8	1069	531	1105	354

Table 5: Number of iterations for different transmission conditions, frequencies values and numbers of sub-domains for the engine compartment problem.

Optimal Interface Condition at the matrix level

When a finite element method, for instance, is used it yields a linear system of the form AU = F, where F is a given right-hand side and U is the set of unknowns.

Corresponding to a domain decomposition, the set of unknowns U is decomposed into interior nodes of the subdomains U_1 and U_2 , and to unknowns, U_{Γ} , associated to the interface Γ . This leads to a block decomposition of the linear system

$$\begin{pmatrix} A_{11} & A_{1\Gamma} & 0 \\ A_{\Gamma 1} & A_{\Gamma\Gamma} & A_{\Gamma 2} \\ 0 & A_{2\Gamma} & A_{22} \end{pmatrix} \begin{pmatrix} U_1 \\ U_{\Gamma} \\ U_2 \end{pmatrix} = \begin{pmatrix} F_1 \\ F_{\Gamma} \\ F_2 \end{pmatrix}.$$
 (6)

Optimal Interface Condition at the matrix level

The DDM method reads:

$$\begin{pmatrix} A_{11} & A_{1\Gamma} \\ A_{\Gamma 1} & A_{\Gamma\Gamma} + S_2 \end{pmatrix} \begin{pmatrix} U_1^{n+1} \\ U_{\Gamma,1}^{n+1} \end{pmatrix} = \begin{pmatrix} F_1 \\ F_{\Gamma} + S_2 U_{\Gamma,2}^n - A_{\Gamma 2} U_2^n \end{pmatrix}$$
(7)

$$\begin{pmatrix} A_{22} & A_{2\Gamma} \\ A_{\Gamma 2} & A_{\Gamma\Gamma} + S_1 \end{pmatrix} \begin{pmatrix} U_2^{n+1} \\ U_{\Gamma,2}^{n+1} \end{pmatrix} = \begin{pmatrix} F_2 \\ F_{\Gamma} + S_1 U_{\Gamma,1}^n - A_{\Gamma 1} U_1^n \end{pmatrix}$$
(8)

where

$$S_1 = -A_{\Gamma 1} A_{11}^{-1} A_{1\Gamma}$$

and

$$S_2 = -A_{\Gamma 2} A_{22}^{-1} A_{2\Gamma}$$

Convergence in two iterations

Approximate Interface Condition at the matrix level

The matrices $S_1 = -A_{\Gamma 1}A_{11}^{-1}A_{1\Gamma}$ and $S_2 = -A_{\Gamma 2}A_{22}^{-1}A_{2\Gamma}$ are full interface matrices $(\Gamma \times \Gamma)$.

Cons

- Costly to compute
- The subdomain matrix is partly full

Approximate S_1 and S_2 by sparse matrices

- 1. e.g. via sparse approximations to A_{ii}^{-1} : SPAI
- 2. via local Schur complements on successive reduced "outer" domains $(\gamma \times \delta)$, "patches", (Roux et al., 2006)

The first approach gives mild results. The second one is not better than using an overlap of depth δ but is cheaper.

Constant coefficient case



Figure 4: Relative residual vs. iteration number for the bicgstab algorithm

Many layers

Very anisotropic and heterogeneous media, $\kappa_M/\kappa_m = 10^7$

Table 2: Gmres solve with $TOL = 10^{-6}$

	Cond. Nb	Iter	$\ e\ $
RAS (Schwarz)	1.9910^{6}	37	3.610^{-2}
Patch	5.2910^5	15	6.110^{-5}
Best IC	2.1	9	1.510^{-7}

Condition number of Patch method is very bad but only one eigenvalue is very small, thus iteration count is good.

More subdomains

The methods generalize to an arbitrary number of subdomains, it is a matter of notations. But, performance may deteriorate with large number of subdomains. Plateaus appear in the convergence of the Krylov methods.



Figure 5: Japhet, Nataf, Roux (1998)

More subdomains

Iteration counts for a Poisson problem on a domain decomposed into strips.

The number of unknowns is proportional to the number of subdomains (scalability).

N subdomains	Schwarz	With coarse grid
4	18	25
8	37	22
16	54	24
32	84	25
64	144	25

More than two subdomains

This corresponds to a few very large (or low) eigenvalues in the spectrum of the substructured problem. They are due to the lack of a global exchange of information in the preconditioner.

Consider with $\eta = 0$:

 $\eta u - \Delta u = f \text{ in } \Omega$ $u = 0 \text{ on } \partial \Omega$



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

A classical remedy consists in the introduction of a coarse grid problem that couples all subdomains. This is closely related to deflation technique classical in linear algebra (see Nabben and Vuik's papers in SIAM J. Sci. Comp).

Domain decomposition based deflation vectors

We denote by Z the deflation vectors. Example for a 3 subdomains decomposition.

$$Z = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \end{pmatrix}$$

and by abuse of notation, we denote by Z the vector space spanned by the columns of Z.

Deflation methods

The original symmetric problem writes $Ax = b \in \mathbb{R}^N$. Let $Z \in \mathbb{R}^{N \times M}$ be formed of M deflation column vectors. Let P be the projection onto Z^T parallel to AZ:

$$P = I_d - AZ(Z^T A Z)^{-1} Z^T$$

Remark that

$$P^T = I_d - Z(Z^T A Z)^{-1} Z^T A$$
 and $PA = A P^T$

We seek x in the form $x = (I_d - P^T)x + P^T x$:

$$A((I_d - P^T)x) = (I_d - P)b$$
 and $PAP^Tx = Pb$.

The first equation corresponds to solving a $M \times M$ problem and the second one can be solved by a preconditioned Krylov method. Details can be found in Nabben and Vuik "A comparison of deflation and the balancing preconditioner." SIAM J. Sci. Comput. (2006).

More subdomains



Figure 6: 64 subdomains

Conclusion

- Both approaches (Neumann-Neumann and optimized Schwarz methods) are robust (thanks to Krylov methods).
- Neumann-Neumann, FETI, .. optimal but lacks generality
- optimized Schwarz methods are general but are more difficult to tune

Open problems

• Theory

Convergence proof or condition number estimate in a general overlapping case

proof of the Non existence of Optimal Interface Conditions for a general domain decomposition

• Algorithm

Algebraic Optimized Interface Conditions

Interplay between the Optimized Interface Conditions and a Coarse Grid

Systems of PDEs (versus scalar PDEs)

Thanks!