# Optimized Schwarz Methods 

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## 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
$\Longrightarrow$ 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 $\Longrightarrow$ need for an "artificial" decomposition

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

Linear Algebra from the End User point of view

$\left.$| Direct Solvers | DDM | Krylov |
| :---: | :---: | :---: |
| Cons: Memory | Pro: Flexible Compromise | Pros: Memory |
| Difficult to parallelize | Parallel computer |  |
| Pros: Robustness |  |  |$\quad$| Easy to parallelize |
| :---: |
| Cons: Robustness | \right\rvert\, | Few black box routines |
| :---: |
| solve(MAT,RHS,SOL) |

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)

$$
\begin{aligned}
& -\Delta(u)=f \quad \text { in } \Omega \\
& u=0 \quad \text { on } \partial \Omega
\end{aligned}
$$

Schwarz Method: $\left(u_{1}^{n}, u_{2}^{n}\right) \rightarrow\left(u_{1}^{n+1}, u_{2}^{n+1}\right)$ with

$$
\begin{array}{ll}
-\Delta\left(u_{1}^{n+1}\right)=f \quad \text { in } \Omega_{1} & -\Delta\left(u_{2}^{n+1}\right)=f \quad \text { in } \Omega_{2} \\
u_{1}^{n+1}=0 \text { on } \partial \Omega_{1} \cap \partial \Omega & u_{2}^{n+1}=0 \text { on } \partial \Omega_{2} \cap \partial \Omega \\
u_{1}^{n+1}=u_{2}^{n} \quad \text { on } \partial \Omega_{1} \cap \overline{\Omega_{2}} . & u_{2}^{n+1}=u_{1}^{n+1} \quad \text { on } \partial \Omega_{2} \cap \overline{\Omega_{1}} .
\end{array}
$$

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

$$
A x=b
$$

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

$$
B x^{n+1}=B x^{n}+\left(b-A x^{n}\right)
$$

Let $r_{0}:=b-A x^{0}$, we have:

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

A preconditioned Krylov solve will generate an optimal $x_{K}^{n}$ in
$\mathcal{K}^{n}\left(B^{-1} A, B^{-1} r_{0}\right):=x_{0}+\operatorname{Span}\left\{B^{-1} r_{0}, B^{-1} A B^{-1} r_{0}, \ldots,\left(B^{-1} A\right)^{n} B^{-1} r_{0}\right\}$ and since $x^{n} \in \mathcal{K}^{n}\left(B^{-1} A, B^{-1} r_{0}\right)$ 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 $\mathcal{N}_{2}$ :

$$
\left(\begin{array}{ll}
A_{11} & A_{12} \\
A_{21} & A_{22}
\end{array}\right)\binom{x_{1}}{x_{2}}=\binom{b_{1}}{b_{2}}
$$

The block-Jacobi algorithm reads:

$$
\left(\begin{array}{cc}
A_{11} & 0 \\
0 & A_{22}
\end{array}\right)\binom{x_{1}^{k+1}}{x_{2}^{k+1}}=-\left(\begin{array}{cc}
0 & A_{12} \\
A_{21} & 0
\end{array}\right)\binom{x_{1}^{k}}{x_{2}^{k}}+\binom{b_{1}}{b_{2}}
$$

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


Figure 1: Domain decomposition with minimal overlap

## Jacobi and Schwarz (II): Larger overlap

Let $\delta$ 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

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

which solves the linear system:

$$
\left(I_{d}-T(\cdot, 0)\right)(x)=T(0, b)
$$

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

$$
\begin{aligned}
& \mathcal{L}(u):=-\Delta(u)=f \quad \text { in } \Omega \\
& u=0 \quad \text { on } \partial \Omega .
\end{aligned}
$$

The domain is decomposed into two non overlapping subdomains. Let $u_{1}$ and $u_{2}$ be the solutions in the subdomains and

$$
\Gamma=\partial \Omega_{1} \cap \partial \Omega_{2}
$$



## First family of modern methods : Substructuring formulation

Consider a non overlapping decomposition of the domain $\Omega$ into $\Omega_{1}$ and $\Omega_{2}$ and Dirichlet BVP in each subdomain with $\left.u\right|_{\Gamma}$ as a Dirichlet data

$$
\begin{aligned}
& -\Delta\left(u_{i}\right)=f \quad \text { in } \Omega_{i}, \\
& u_{i}=\left.u\right|_{\Gamma} \quad \text { on } \Gamma, \quad u_{i}=0 \quad \operatorname{sur} \partial \Omega_{i} \backslash \Gamma .
\end{aligned}
$$

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

$$
\mathcal{S}\left(f,\left.u\right|_{\Gamma}\right)=\left.\frac{1}{2}\left(\frac{\partial u_{1}}{\partial n_{1}}+\frac{\partial u_{2}}{\partial n_{2}}\right)\right|_{\Gamma}
$$

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

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

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

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


## 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 $\mathcal{T}$ :

$$
\begin{aligned}
& \mathcal{T}: H^{-\frac{1}{2}}(\Gamma) \rightarrow H_{00}^{\frac{1}{2}}(\Gamma) \\
& \mathcal{T}(g)=\left.\frac{1}{2}\left(v_{1}+v_{2}\right)\right|_{\Gamma} .
\end{aligned}
$$

where

$$
\begin{array}{ll}
\mathcal{L} v_{i}=0 & \text { in } \Omega_{i}, \\
\frac{\partial v_{i}}{\partial n_{i}}=g & \text { sur } \Gamma
\end{array}
$$

## Optimality

The preconditioned operator $\mathcal{T} \mathcal{S}(0,$.$) is a continuous operator from$ $H_{00}^{\frac{1}{2}} \rightarrow H_{00}^{\frac{1}{2}}$. 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

$$
\begin{aligned}
& \mathcal{L}\left(u_{i}\right)=f \quad \text { in } \Omega_{i}, \\
& \frac{\partial u_{i}}{\partial n_{i}}=\left.(-1)^{i+1} \lambda\right|_{\Gamma} \quad \text { on } \Gamma \\
& u_{i}=0 \quad \text { sur } \partial \Omega_{i} \backslash \Gamma .
\end{aligned}
$$

We consider the Neuman to Dirichlet (NtD) map

$$
\begin{aligned}
& \mathcal{T}_{\text {feti }}: L^{2}(\Omega) \times H^{-\frac{1}{2}}(\Gamma) \rightarrow H_{00}^{\frac{1}{2}}(\Gamma) \\
& \mathcal{T}_{\text {feti }}\left(f,\left.\lambda\right|_{\Gamma}\right)=\left.\frac{1}{2}\left(u_{1}-u_{2}\right)\right|_{\Gamma}
\end{aligned}
$$

The substructured problem reads:

$$
\mathcal{T}_{\text {feti } i}\left(0,\left.\lambda\right|_{\Gamma}\right)=-\mathcal{T}_{\text {feti } i}(f, 0)
$$

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)

$$
\begin{aligned}
& -\Delta\left(u_{1}^{n+1}\right)=f \quad \text { in } \Omega_{1}, \\
& u_{1}^{n+1}=0 \quad \text { on } \partial \Omega_{1} \cap \partial \Omega \\
& \left(\frac{\partial}{\partial n_{1}}+\alpha\right)\left(u_{1}^{n+1}\right)=\left(-\frac{\partial}{\partial n_{2}}+\alpha\right)\left(u_{2}^{n}\right) \quad \text { on } \partial \Omega_{1} \cap \overline{\Omega_{2}},
\end{aligned}
$$

( $n_{1}$ and $n_{2}$ are the outward normal on the boundary of the subdomains)

$$
\begin{aligned}
& -\Delta\left(u_{2}^{n+1}\right)=f \quad \text { in } \Omega_{2}, \\
& u_{2}^{n+1}=0 \quad \text { on } \partial \Omega_{2} \cap \partial \Omega \\
& \left(\frac{\partial}{\partial n_{2}}+\alpha\right)\left(u_{2}^{n+1}\right)=\left(-\frac{\partial}{\partial n_{1}}+\alpha\right)\left(u_{1}^{n}\right) \quad \text { on } \partial \Omega_{2} \cap \overline{\Omega_{1}} .
\end{aligned}
$$

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)

$$
\begin{aligned}
& -\Delta\left(u_{1}^{n+1}\right)=f \quad \text { in } \Omega_{1} \\
& u_{1}^{n+1}=0 \quad \text { on } \partial \Omega_{1} \cap \partial \Omega \\
& \left(\frac{\partial}{\partial n_{1}}+\alpha\right)\left(u_{1}^{n+1}\right)=\left(-\frac{\partial}{\partial n_{2}}+\alpha\right)\left(u_{2}^{n}\right) \quad \text { on } \partial \Omega_{1} \cap \overline{\Omega_{2}},
\end{aligned}
$$

( $n_{1}$ and $n_{2}$ are the outward normal on the boundary of the subdomains)

$$
\begin{aligned}
& -\Delta\left(u_{2}^{n+1}\right)=f \quad \text { in } \Omega_{2}, \\
& u_{2}^{n+1}=0 \quad \text { on } \partial \Omega_{2} \cap \partial \Omega \\
& \left(\frac{\partial}{\partial n_{2}}+\alpha\right)\left(u_{2}^{n+1}\right)=\left(-\frac{\partial}{\partial n_{1}}+\alpha\right)\left(u_{1}^{n}\right) \quad \text { on } \partial \Omega_{2} \cap \overline{\Omega_{1}} .
\end{aligned}
$$

with $\alpha>0$. Overlap is not necessary for convergence.
Extended to the Helmholtz equation (B. Desprès, 1991)
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## 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.

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

with $\eta(\mathbf{x}), \kappa(\mathbf{x})>C>0$. The domain is decomposed into $N$ subdomains $\left(\Omega_{i}\right)_{1 \leq i \leq N}$ without overlap.
Let $\Gamma_{i j}$ denote the interface $\Gamma_{i j}=\partial \Omega_{i} \cap \partial \Omega_{j}$.

## Convergence

The interface condition is

$$
\begin{aligned}
\kappa(\mathbf{x}) \frac{\partial u_{i}^{n+1}}{\partial n_{i}}+\alpha_{i j}(\mathbf{x}) & u_{i}^{n+1}-\frac{\partial}{\partial \tau_{i}}\left(\gamma_{i j}(\mathbf{x}) \frac{\partial u_{i}^{n+1}}{\partial \tau_{i}}\right) \\
& =-\kappa(\mathbf{x}) \frac{\partial u_{j}^{n}}{\partial n_{j}}+\alpha_{i j}(\mathbf{x}) u_{j}^{n}-\frac{\partial}{\partial \tau_{j}}\left(\gamma_{i j}(\mathbf{x}) \frac{\partial u_{j}^{n}}{\partial \tau_{j}}\right) \text { on } \Gamma_{i j}
\end{aligned}
$$

with

$$
\begin{gathered}
\alpha_{i j}(\mathbf{x})=\alpha_{j i}(\mathbf{x}) \geq \alpha_{0}>0 \\
\gamma(\mathbf{x})_{i j}=\gamma(\mathbf{x})_{j i} \geq 0 \text { et } \gamma_{i j}(\mathbf{x})=0 \text { sur } \partial \Gamma_{i j}
\end{gathered}
$$

Let us denote

$$
\Lambda_{i j}=\alpha_{i j}(\mathbf{x})-\frac{\partial}{\partial \tau_{i}}\left(\gamma_{i j}(\mathbf{x}) \frac{\partial}{\partial \tau_{i}}\right), \quad \mathbf{x} \in \Gamma_{i j}
$$

Lemma 1 The algorithm converges in $H^{1}$ (discrete norm).
The convergence rate is very sensitive to $\alpha$ and $\gamma$, how to choose them?

## Optimal Interface Conditions

(Hagstrom, 1988)
Constant coefficient Advection-Diffusion equation on a domain decomposed into two subdomains.

$$
\begin{aligned}
& (\vec{a} \nabla-\nu \Delta)\left(u_{1}^{n+1}\right)=f \quad \text { in } \Omega_{1}, \\
& u_{1}^{n+1}=0 \quad \text { on } \partial \Omega_{1} \cap \partial \Omega, \\
& \left(\frac{\partial}{\partial n_{1}}+\mathcal{B}_{1}\right)\left(u_{1}^{n+1}\right)=\left(-\frac{\partial}{\partial n_{2}}+\mathcal{B}_{1}\right)\left(u_{2}^{n}\right) \\
& \\
& (\vec{a} \nabla-\nu \Delta)\left(u_{2}^{n+1}\right)=f \quad \text { on } \partial \Omega_{1} \cap \overline{\Omega_{2}}, \\
& u_{2}^{n+1}=0 \quad \text { on } \partial \Omega_{2} \cap \partial \Omega \\
& \left(\frac{\partial}{\partial n_{2}}+\mathcal{B}_{2}\right)\left(u_{2}^{n+1}\right)=\left(-\frac{\partial}{\partial n_{1}}+\mathcal{B}_{2}\right)\left(u_{1}^{n}\right) \\
& \text { on } \partial \Omega_{2} \cap \overline{\Omega_{1}} .
\end{aligned}
$$

where $\mathcal{B}_{i}, i=1,2$ are defined via a Fourier transform along the interface
Convergence in two iterations

## Optimal Interface Conditions

Let us consider the problem

$$
\begin{array}{ll}
\mathcal{L}_{i}\left(P_{i}\right) \quad \text { in } \Omega_{i}, & i=1,2 \\
P_{1}=P_{2} \quad \text { on } \Gamma_{12}, & \\
\kappa_{1} \frac{\partial P_{1}}{\partial n_{1}}+\kappa_{2} \frac{\partial P_{2}}{\partial n_{2}}=0 & \text { on } \Gamma_{12} .
\end{array}
$$

where

$$
\mathcal{L}_{i}=\eta_{i}-\operatorname{div}\left(\kappa_{i} \nabla \dot{)}\right.
$$

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

## Optimal Interface Conditions

Let

$$
u_{i}=\kappa_{i} \nabla P_{i}
$$

Let us consider a Schwarz type method:

$$
\begin{array}{ll}
\mathcal{L}_{1}\left(P_{1}^{n+1}\right)=f \quad \text { in } \Omega_{1} & \mathcal{L}_{2}\left(P_{2}^{n+1}\right)=f \quad \text { in } \Omega_{2} \\
P_{1}^{n+1}=0 \text { on } \partial \Omega_{1} \cap \partial \Omega & P_{2}^{n+1}=0 \text { on } \partial \Omega_{2} \cap \partial \Omega \\
u_{1}^{n+1} \cdot \vec{n}_{1}+\mathcal{B}_{1}\left(P_{1}^{n+1}\right) & u_{2}^{n+1} \cdot \vec{n}_{2}+\mathcal{B}_{2}\left(P_{2}^{n+1}\right) \\
=-u_{2}^{n} \cdot \vec{n}_{2}+\mathcal{B}_{1}\left(P_{2}^{n}\right) \quad \text { on } \Gamma_{1} & =-u_{1}^{n} \cdot \vec{n}_{1}+\mathcal{B}_{2}\left(P_{1}^{n}\right) \quad \text { on } \Gamma_{2}
\end{array}
$$

We take

$$
\mathcal{B}_{1}=D t N_{2} .
$$

and have convergence in two iterations.

## Optimal Interface Conditions

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

$$
\begin{align*}
& \text { Let } P_{0}: \Gamma_{12} \rightarrow \mathbb{R}  \tag{1}\\
& \operatorname{DtN} N_{2}\left(P_{0}\right) \equiv \kappa_{2} \frac{\partial}{\partial n_{2}}(P)_{\mid \Gamma_{12}}
\end{align*}
$$

where $n_{2}$ is the outward normal to $\Omega_{2} \backslash \bar{\Omega}_{1}$ and $P$ satisfies the following boundary value problem:

$$
\begin{aligned}
& \mathcal{L}(P)=0 \text { in } \Omega_{2} \\
& P=0 \text { on } \partial \Omega_{2} \backslash \Gamma_{i} \\
& P=P_{0} \text { on } \Gamma_{12} .
\end{aligned}
$$

We take

$$
\mathcal{B}_{1}=D t N_{2}
$$

## Optimal Interface Conditions

(Rogier, de Sturler and N., 1993)
The result can be generalized to variable coefficients operators and a decomposition of the domain $\Omega$ 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 $D t N$ 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

$$
D t N \simeq \alpha_{o p t}-\frac{\partial}{\partial \tau}\left(\gamma_{o p t} \frac{\partial}{\partial \tau}\right)
$$

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 $\alpha$, 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:

$$
\begin{aligned}
& \left.\mathcal{L}\left(u_{1}^{n+1}\right)=f \quad \text { in } \Omega_{1}:=\right]-\infty, \delta[\times \mathbb{R}, \\
& \left(\frac{\partial}{\partial n_{1}}+\alpha\right)\left(u_{1}^{n+1}\right)=\left(-\frac{\partial}{\partial n_{2}}+\alpha\right)\left(u_{2}^{n}\right) \quad \text { at } x=\delta \\
& \left.\mathcal{L}\left(u_{2}^{n+1}\right)=f \quad \text { in } \Omega_{2}:=\right] 0, \infty[\times \mathbb{R}, \\
& \left(\frac{\partial}{\partial n_{2}}+\alpha\right)\left(u_{2}^{n+1}\right)=\left(-\frac{\partial}{\partial n_{1}}+\alpha\right)\left(u_{1}^{n}\right) \quad \text { at } x=0
\end{aligned}
$$

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:

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

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

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

$$
\rho\left(\alpha_{o p t}\right):=\min _{\alpha>0} \max _{|k| \leq 1 / h} \rho(k ; 0, \alpha)
$$

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

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

| $1 / \Delta y$ | 10 | 20 | 40 | 80 |
| :---: | :---: | :---: | :---: | :---: |
| $\alpha_{\mathrm{opt}}^{\mathrm{sc}}$ | 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 $\alpha$, no overlap

## Application: the Helmholtz Equation

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

We want to solve

$$
\begin{aligned}
& -\omega^{2} u-\Delta u=f \quad \text { in } \Omega \\
& u=0 \quad \text { on } \partial \Omega
\end{aligned}
$$

The relaxation algorithm is : $\left(u_{1}^{p}, u_{2}^{p}\right) \rightarrow\left(u_{1}^{p+1}, u_{2}^{p+1}\right)$ with $(i \neq j, i=1,2)$

$$
\begin{aligned}
& \left(-\omega^{2}-\Delta\right)\left(u_{i}^{p+1}\right)=f \quad \text { in } \Omega_{i} \\
& \left(\frac{\partial}{\partial n_{i}}+\mathcal{S}\right)\left(u_{i}^{p+1}\right)=\left(-\frac{\partial}{\partial n_{j}}+\mathcal{S}\right)\left(u_{j}^{p}\right) \quad \text { on } \Gamma_{i j} \\
& u_{i}^{p+1}=0 \text { on } \partial \Omega_{i} \cap \partial \Omega
\end{aligned}
$$

The operator $\mathcal{S}$ has the form

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

## Application: the Helmholtz Equation

By choosing carefully the coefficients $\alpha$ and $\gamma$, it is possible to optimize the convergence rate of the iterative method which in the Fourier space is given by

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

Finally, we get analytic formulas for $\alpha$ and $\gamma$ ( $h$ is the mesh size):

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

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 $\mathrm{ABC0}\left(\partial_{n}+I \omega\right)$ with relaxation on the interface


Chevalier and N., 1997

## 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

$$
\lambda^{1}=-\frac{\partial u_{2}}{\partial n_{2}}+\mathcal{S}\left(u_{2}\right) \text { and } \lambda^{2}=-\frac{\partial u_{1}}{\partial n_{1}}+\mathcal{S}\left(u_{1}\right) .
$$

The algorithm reads now

$$
\begin{array}{r}
-\Delta u_{1}^{n+1}+\omega^{2} u_{1}^{n+1}=f \text { in } \Omega_{1} \\
\frac{\partial u_{1}^{n+1}}{\partial n_{1}}+\mathcal{S}\left(u_{1}^{n+1}\right)=\lambda^{1^{n}} \text { on } \Gamma_{12} \\
-\Delta u_{2}^{n+1}+\omega^{2} u_{2}^{n+1}=f \text { in } \Omega_{2} \\
\frac{\partial u_{2}^{n+1}}{\partial n_{2}}+\mathcal{S}\left(u_{2}^{n+1}\right)=\lambda^{2^{n}} \text { on } \Gamma_{12} \\
\lambda^{1^{n+1}}=-\lambda^{2^{n}}+(\mathcal{S}+\mathcal{S})\left(u_{2}^{n+1}\left(\lambda^{1^{p}}, f\right)\right) \\
\lambda^{2^{n+1}}=-\lambda^{1^{n}}+(\mathcal{S}+\mathcal{S})\left(u_{1}^{n+1}\left(\lambda^{2^{p}}, f\right)\right)
\end{array}
$$

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:

$$
\begin{align*}
\lambda^{1} & =-\lambda^{2}+(S+S) B^{2} u^{2} \\
\lambda^{2} & =-\lambda^{1}+(S+S) B^{1} u^{1} \\
\widetilde{K}^{1} u^{1} & =f^{1}+{B^{1^{T}} \lambda^{1}}_{\widetilde{K}^{2} u^{2}}=f^{2}+B^{2^{T}} \lambda^{2}
\end{align*}
$$

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

$$
\begin{equation*}
\widetilde{K}^{i}=K^{i}-\omega^{2} M^{i}+B^{i^{T}}\left(\alpha M_{\Gamma_{12}}+\gamma K_{\Gamma_{12}}\right) B^{i} \tag{3}
\end{equation*}
$$

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

$$
\begin{equation*}
\left[M_{\Gamma_{12}}\right]_{l m}=\int_{\Gamma_{12}} \phi_{l} \phi_{m} d \xi \text { and }\left[K_{\Gamma_{12}}\right]_{l m}=\int_{\Gamma_{12}} \nabla_{\tau} \phi_{l} \nabla_{\tau} \phi_{m} d \xi \tag{4}
\end{equation*}
$$

where $\phi_{l}$ et $\phi_{m}$ are the basis functions associated to nodes $l$ and $m$ on the interface $\Gamma_{12}$ 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

$$
\begin{equation*}
F \lambda=d \tag{5}
\end{equation*}
$$

where $\lambda=\left(\lambda^{1}, \lambda^{2}\right), F$ is a matrix and $d$ is the right handside

$$
\begin{aligned}
F & =\left[\begin{array}{cc}
I & I-(S+S) B^{2} \widetilde{K}^{2^{-1}} B^{2^{T}} \\
I-(S+S) B^{1} \widetilde{K}^{1^{-1}} B^{1^{T}} & I
\end{array}\right] \\
d & =\left[\begin{array}{c}
(S+S) B^{1} \widetilde{K}^{1^{-1}} f^{1} \\
(S+S) B^{2} \widetilde{K}^{2^{-1}} f^{2}
\end{array}\right]
\end{aligned}
$$

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 $\left(\partial_{n}+I \omega\right)$ 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 $0\left(\partial_{n}+I \omega\right)$
ABC 2: Absorbing Boundary Conditions of Order 2
$\left(\partial_{n}+I \omega-1 /(2 I \omega) \partial_{y^{2}}\right)$
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 $A U=F$, 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, $U_{\Gamma}$, associated to the interface $\Gamma$. This leads to a block decomposition of the linear system

$$
\left(\begin{array}{ccc}
A_{11} & A_{1 \Gamma} & 0  \tag{6}\\
A_{\Gamma 1} & A_{\Gamma \Gamma} & A_{\Gamma 2} \\
0 & A_{2 \Gamma} & A_{22}
\end{array}\right)\left(\begin{array}{l}
U_{1} \\
U_{\Gamma} \\
U_{2}
\end{array}\right)=\left(\begin{array}{c}
F_{1} \\
F_{\Gamma} \\
F_{2}
\end{array}\right) .
$$

## Optimal Interface Condition at the matrix level

The DDM method reads:

$$
\begin{align*}
& \left(\begin{array}{cc}
A_{11} & A_{1 \Gamma} \\
A_{\Gamma 1} & A_{\Gamma \Gamma}+S_{2}
\end{array}\right)\binom{U_{1}^{n+1}}{U_{\Gamma, 1}^{n+1}}=\binom{F_{1}}{F_{\Gamma}+S_{2} U_{\Gamma, 2}^{n}-A_{\Gamma 2} U_{2}^{n}}  \tag{7}\\
& \left(\begin{array}{cc}
A_{22} & A_{2 \Gamma} \\
A_{\Gamma 2} & A_{\Gamma \Gamma}+S_{1}
\end{array}\right)\binom{U_{2}^{n+1}}{U_{\Gamma, 2}^{n+1}}=\binom{F_{2}}{F_{\Gamma}+S_{1} U_{\Gamma, 1}^{n}-A_{\Gamma 1} U_{1}^{n}} \tag{8}
\end{align*}
$$

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 $A_{i i}^{-1}$ : 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 $\delta$ 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 $T O L=10^{-6}$

|  | 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 $\eta=0$ :

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



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.

$$
Z=\left(\begin{array}{c|c|c}
1 & 0 & 0 \\
1 & 0 & 0 \\
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1 \\
0 & 0 & 1 \\
0 & 0 & 1
\end{array}\right)
$$

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 $A x=b \in \mathbb{R}^{N}$.
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 $A Z$ :

$$
P=I_{d}-A Z\left(Z^{T} A Z\right)^{-1} Z^{T}
$$

Remark that

$$
P^{T}=I_{d}-Z\left(Z^{T} A Z\right)^{-1} Z^{T} A \text { and } P A=A P^{T}
$$

We seek $x$ in the form $x=\left(I_{d}-P^{T}\right) x+P^{T} x$ :

$$
A\left(\left(I_{d}-P^{T}\right) x\right)=\left(I_{d}-P\right) b \text { and } P A P^{T} x=P b .
$$

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!

