Adaptive optimized Schwarz methods

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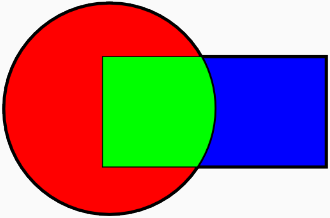
Brief history of domain decomposition

H.A. Schwarz, 1869

How do we solve the Laplace equation on complicated domains?

We split the domain into simpler subdomains.



Alternating Schwarz method:

$$\begin{cases} \Delta u_1^{n+1} = 0 & \text{in } \Omega_1, \\ u_1^{n+1} = u_2^n & \text{on } \Gamma_1, \end{cases} \qquad \begin{cases} \Delta u_2^{n+1} = 0 & \text{in } \Omega_2, \\ u_2^{n+1} = u_1^{n+1} & \text{on } \Gamma_2. \end{cases}$$

P.L. Lions, 1989

Parallel Schwarz method:

$$\begin{cases} \Delta u_1^{n+1} = 0 & \text{in } \Omega_1, \\ u_1^{n+1} = u_2^n & \text{on } \Gamma_1, \end{cases} \quad \begin{cases} \Delta u_2^{n+1} = 0 & \text{in } \Omega_2, \\ u_2^{n+1} = u_1^n & \text{on } \Gamma_2. \end{cases}$$

Multiple subdomains:

$$\begin{cases} \Delta u_i^{n+1} = 0 & \text{in } \Omega_i, \\ u_i^{n+1} = u_j^n & \text{on } \Gamma_{ij} \end{cases}$$

where Γ_{ij} is the boundary of Ω_i that lies in Ω_j.

Algebraic domain decomposition

$$A\boldsymbol{u} = \begin{bmatrix} A_{11} & A_{1\Gamma} & \\ A_{\Gamma 2} & A_{\Gamma\Gamma} & A_{\Gamma 1} \\ & A_{2\Gamma} & A_{22} \end{bmatrix} \begin{bmatrix} \boldsymbol{u}_1 \\ \boldsymbol{u}_\Gamma \\ \boldsymbol{u}_2 \end{bmatrix} = \begin{bmatrix} \boldsymbol{f}_1 \\ \boldsymbol{f}_\Gamma \\ \boldsymbol{f}_2 \end{bmatrix} = \boldsymbol{f}$$

The domain Ω is split into Ω_1, which contains the variables in $\boldsymbol{u}_1$ and $\boldsymbol{u}_\Gamma$, and Ω_2, which contains the variables in $\boldsymbol{u}_2$ and $\boldsymbol{u}_\Gamma$.

The variables $\boldsymbol{u}_\Gamma$ are shared between the two subdomains and forms an **interface** between the two.

Algebraic Schwarz methods

The two subdomains in algebraic Schwarz are

$$\begin{bmatrix} A_{11} & A_{1\Gamma} \\ A_{\Gamma 1} & A_{\Gamma\Gamma} + T_{2\to 1} \end{bmatrix} \begin{bmatrix} \boldsymbol{u}_1^{n+1} \\ \boldsymbol{u}_{1\Gamma}^{n+1} \end{bmatrix} = \begin{bmatrix} \boldsymbol{f}_1 \\ \boldsymbol{f}_\Gamma \end{bmatrix} + \begin{bmatrix} \\ -A_{\Gamma 2}\boldsymbol{u}_2^n + T_{2\to 1}\boldsymbol{u}_{2\Gamma}^n \end{bmatrix},$$

$$\begin{bmatrix} A_{22} & A_{2\Gamma} \\ A_{\Gamma 2} & A_{\Gamma\Gamma} + T_{1\to 2} \end{bmatrix} \begin{bmatrix} \boldsymbol{u}_2^{n+1} \\ \boldsymbol{u}_{2\Gamma}^{n+1} \end{bmatrix} = \begin{bmatrix} \boldsymbol{f}_2 \\ \boldsymbol{f}_\Gamma \end{bmatrix} + \begin{bmatrix} \\ -A_{\Gamma 1}\boldsymbol{u}_1^n + T_{1\to 2}\boldsymbol{u}_{1\Gamma}^n \end{bmatrix},$$

for any choice of matrices $T_{1\to 2}$ and $T_{2\to 1}$ (that does not make these systems singular).

Each choice of matrices T corresponds to a choice of boundary conditions on the interface, called **transmission conditions**, since they transmit information between subdomains.

Options for transmission conditions

- Dirichlet boundary conditions, equivalent to $T = 0$
- Neumann boundary conditions, allow minimal overlap
- Optimized Robin boundary conditions:

$$\frac{\partial u_1^{n+1}}{\partial x} - p u_1^{n+1} = \frac{\partial u_2^n}{\partial x} - p u_2^n$$

  for some p optimized using Fourier analysis
- Absorbing boundary conditions, equivalent to Schur complements:

$$S_{i \to j} := -A_{\Gamma i} A_{ii}^{-1} A_{i\Gamma}$$

With absorbing boundary conditions, the method becomes direct. However, the Schur complements are expensive to compute and in general dense.

Schwarz as a fixed point iteration

Schwarz methods can be represented as fixed point iterations:

$$u^{n+1} = g\left(u^{n-1}\right),$$

where $g(u)$ represents one iteration of a Schwarz method that takes boundary data from the input u.

The fixed point of g is the solution on the first subdomain. This is also the root of the function $f(u) = g(u) - u$. We apply Newton's method:

$$u^{*} = u^{n-1} - J(u^{n-1})^{-1} f(u^{n-1}),$$

where J is the Jacobian of the function f.

Schwarz-Preconditioned Newton methods (Cai & Keyes, 2001)

This is equivalent to preconditioning Newton's method with a Schwarz method.

Let

$$f(u) = \begin{bmatrix} f_1(u_1, u_2) \\ f_2(u_1, u_2) \end{bmatrix}.$$

Then Newton's method tells us to solve the nonlinear problem

$$\begin{bmatrix} J_{11}^{(n+1)} & J_{12}^{(n+1)} \\ J_{21}^{(n+1)} & J_{22}^{(n+1)} \end{bmatrix} \begin{bmatrix} u_1^{n+1} - u_1^n \\ u_2^{n+1} - u_2^n \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \end{bmatrix},$$

where $J_{ij}^{(n+1)}$ is the derivative of f_i with respect to u_j evaluated at u_1^{n+1} and u_2^{n+1}.

Schwarz-Preconditioned Newton methods (Cai & Keyes, 2001)

Preconditioning this with a parallel Schwarz method tells us to solve

$$\begin{bmatrix} J_{11}^{(n+1)} & \\ & J_{22}^{(n+1)} \end{bmatrix} \begin{bmatrix} u_1^{n+1} - u_1^n \\ u_2^{n+1} - u_2^n \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \end{bmatrix} - \begin{bmatrix} & J_{12}^{(n)} \\ J_{21}^{(n)} & \end{bmatrix} \begin{bmatrix} u_1^n - u_1^{n-1} \\ u_2^n - u_2^{n-1} \end{bmatrix},$$

and completing the iteration by solving

$$\begin{bmatrix} J_{11}^{(n+1)} & \\ & J_{22}^{(n+1)} \end{bmatrix}^{-1} \begin{bmatrix} J_{11}^{(n+1)} & J_{12}^{(n+1)} \\ J_{21}^{(n+1)} & J_{22}^{(n+1)} \end{bmatrix} \begin{bmatrix} u_1^* - u_1^n \\ u_2^* - u_2^n \end{bmatrix} = \begin{bmatrix} f_1(u_1^{n+1}, u_2^{n+1}) \\ f_2(u_1^{n+1}, u_2^{n+1}) \end{bmatrix}.$$

Alternate minimization in phase-field fracture models

Adaptive optimized Schwarz methods

Schwarz method with adaptive transmission conditions

Let $T_{i\to j}$ change at each iteration, so that the transmission conditions adapt. We can formulate such a Schwarz method, acting only on the difference in successive solutions,n as

$$\begin{bmatrix} A_{ii} & A_{i\Gamma} \\ A_{\Gamma i} & A_{\Gamma\Gamma} + T_{j\to i}^{n+1} \end{bmatrix} \begin{bmatrix} \boldsymbol{d}_i^{n+1} \\ \boldsymbol{d}_{i\Gamma}^{n+1} \end{bmatrix} = \begin{bmatrix} \\ -A_{\Gamma j}\boldsymbol{d}_j^n + T_{j\to i}^{n+1}\boldsymbol{d}_{j\Gamma}^n \end{bmatrix} - \begin{bmatrix} \\ \Delta T_{j\to i}^n \left(\boldsymbol{u}_{i\Gamma}^n - \boldsymbol{u}_{j\Gamma}^{n-1}\right) \end{bmatrix},$$

where $i = 1, 2$, $j = 3 - i$, and $\Delta T_{j\to i}^n$ represents the update to the transmission condition $T_{j\to i}^n$ at this step,

$$T_{j\to i}^{n+1} = T_{j\to i}^n + \Delta T_{j\to i}^n.$$

Condensing the iteration

We can condense these iterations to express them as only acting on the difference at the interface. First we note from the first row of blocks that

$$\boldsymbol{d}_i^{n+1} = -A_{ii}^{-1} A_{i\Gamma} \boldsymbol{d}_{i\Gamma}^{n+1},$$

and so likewise

$$\boldsymbol{d}_j^{n} = -A_{jj}^{-1} A_{j\Gamma} \boldsymbol{d}_{j\Gamma}^{n}.$$

Combining with the second row of blocks gives

$$\begin{aligned} \left(A_{\Gamma\Gamma} + S_{i\to j} + T_{j\to i}^{n+1}\right) \boldsymbol{d}_{i\Gamma}^{n+1} = {} & \left(T_{j\to i}^{n+1} - S_{j\to i}\right) \boldsymbol{d}_{j\Gamma}^{n} \\ & - \Delta T_{j\to i}^{n} \left(\boldsymbol{u}_{i\Gamma} - \boldsymbol{u}_{j\Gamma}^{n-1}\right). \end{aligned}$$

Difference between T and S

Notice the difference between the T matrices and the Schur complements in these systems. If we represent this difference as

$$E_{i\to j}^{n+1} := T_{i\to j}^{n+1} - S_{i\to j},$$

and write $\hat{A} := A_{\Gamma\Gamma} + S_{1\to 2} + S_{2\to 1}$, then these systems become

$$\left(\hat{A} + E_{i\to j}^{n+1}\right) \boldsymbol{d}_{j\Gamma}^{n+1} = E_{i\to j}^{n+1} \boldsymbol{d}_{i\Gamma}^{n} - \Delta T_{i\to j}^{n} \left(\boldsymbol{u}_{j\Gamma}^{n} - \boldsymbol{u}_{i\Gamma}^{n-1}\right).$$

The matrix $E_{i\to j}^{n+1}$ is as expensive to calculate as the Schur complement, meaning this system is not practical. However, it has immense theoretical value.

Action of E

The matrix-vector product $E_{i\to j}^{n+1}\boldsymbol{d}_{i\Gamma}^{n}$, equal to

$$E_{i\to j}^{n+1}\boldsymbol{d}_{i\Gamma}^{n} = -A_{\Gamma i}\boldsymbol{d}_{i}^{n} + T_{i\to j}^{n+1}\boldsymbol{d}_{i\Gamma}^{n},$$

is computed in the course of the Schwarz method. Thus, we will have a sequence of vector pairs, $\left(\boldsymbol{d}_{i\Gamma}^{n}, E_{i\to j}^{n+1}\boldsymbol{d}_{i\Gamma}^{n}\right)$ which we can use to approximate E without ever calculating it.

Each vector pair gives a rank one approximation of E:

$$E_{i\to j}^{n+1} \approx \frac{E_{i\to j}^{n+1}\boldsymbol{d}_{i\Gamma}^{n}}{\left\|\boldsymbol{d}_{i\Gamma}^{n}\right\|_2^2}.$$

To combine these rank one matrices, we apply **modified Gram-Schmidt** to the vectors $\boldsymbol{d}$ and a commenserate process to the vectors $E\boldsymbol{d}$.

Algorithm 1 Iterative action approximation

$[V_n, W_n] = \mathrm{IAA}\left(\{\boldsymbol{x}_k\}_{k=1}^{n}, E\right)$

Inputs: $\{\boldsymbol{x}_k\}_{k=1}^{n} \subset \mathbb{R}^M$, $E \in \mathbb{R}^{M\times M}$

$\alpha_1 := 1/\left\|\boldsymbol{x}_1\right\|$, $\boldsymbol{w}_1 := \alpha_1 \boldsymbol{x}_1$, $\boldsymbol{v}_1 := \alpha_1 E \boldsymbol{x}_1$

for $k = 2 : n$ **do**

    $\boldsymbol{w}_k := \boldsymbol{x}_k$, $\boldsymbol{v}_k := E\boldsymbol{x}_k$

    for $i = 1 : k-1$ **do**

        $h \leftarrow \langle \boldsymbol{w}_i, \boldsymbol{w}_k \rangle$, $\boldsymbol{w}_k \leftarrow \boldsymbol{w}_k - h\boldsymbol{w}_i$

        $\boldsymbol{v}_k \leftarrow \boldsymbol{v}_k - h\boldsymbol{v}_i$

    end for

    $\alpha_k := 1/\left\|\boldsymbol{w}_k\right\|$, $\boldsymbol{w}_k \leftarrow \alpha_k \boldsymbol{w}_k$, $\boldsymbol{v}_k \leftarrow \alpha_k \boldsymbol{v}_k$

end for

Outputs: $W_n = \begin{bmatrix} \boldsymbol{w}_1 & \boldsymbol{w}_2 & \dots & \boldsymbol{w}_n \end{bmatrix}$, $V_n = \begin{bmatrix} \boldsymbol{v}_1 & \boldsymbol{v}_2 & \dots & \boldsymbol{v}_n \end{bmatrix}$

$V_n W_n^\top \approx E$

Properties of the IAA

Lemma

Let $\mathcal{S} = \{\boldsymbol{x}_k\}_{k=1}^{n} \subset \mathbb{R}^M$ *be a set of linearly independent vectors,* $E \in \mathbb{R}^{M \times M}$ *a matrix. Let* $[V_n, W_n] = \mathrm{IAA}(\mathcal{S}, E)$ *with columns* $\boldsymbol{v}_k$ *and* $\boldsymbol{w}_k$*, respectively. Let* $E^1 := E$ *and let* $E^{k+1} := E^k - \boldsymbol{v}_k \boldsymbol{w}_k^\top$*. Then*

$$\begin{aligned} E^{k+1} &= E(I - W_k W_k^\top), \\ \boldsymbol{v}_k &= E\boldsymbol{w}_k = E^k \boldsymbol{w}_k \end{aligned}$$

for $1 \leq k \leq n$*, where* W_k *is the first* k *columns of* W_n*.*

Choice of adaptive transmission conditions

For our adaptive transmission conditions, we want

$$[V_i^n, W_i^n] = \mathrm{IAA}\left(\left\{\boldsymbol{d}_{i\Gamma}^k\right\}_{k=1}^n, E_{i\to j}^1\right),$$

$$\text{where } E_{i\to j}^1 \boldsymbol{d}_{i\Gamma}^k = -A_{\Gamma i}\boldsymbol{d}_i^k + T_{i\to j}^1 \boldsymbol{d}_{i\Gamma}^k.$$

Each time we find a new $\boldsymbol{d}_{i\Gamma}^k$, with corresponding $\boldsymbol{d}_i^k$, we can compute a new $\boldsymbol{v}_i^k$ and $\boldsymbol{w}_i^k$. This gives us a rank one update to the transmission conditions:

$$\Delta T_{i\to j}^n = -\boldsymbol{v}_i^k \left(\boldsymbol{w}_i^k\right)^\top.$$

This choice of ΔT eliminates the product $E_{i\to j}^{n+1}\boldsymbol{d}_{i\Gamma}^n$ from the earlier systems. We must now solve

$$\begin{bmatrix} A_{jj} & A_{j\Gamma} \\ A_{\Gamma j} & A_{\Gamma\Gamma} + T_{i\to j}^{n+1} \end{bmatrix} \begin{bmatrix} \boldsymbol{d}_j^{n+1} \\ \boldsymbol{d}_{j\Gamma}^{n+1} \end{bmatrix} = \left(\boldsymbol{w}_i^n\right)^\top \left(\boldsymbol{u}_{j\Gamma}^n - \boldsymbol{u}_{i\Gamma}^{n-1}\right) \begin{bmatrix} \\ \boldsymbol{v}_i^n \end{bmatrix}$$

at every step.

Algorithm 2 altAOSM: AOSM applied to multiplicative Schwarz

Start with initial transmission conditions $T^1_{1\to 2}$ and $T^1_{2\to 1}$

Make initial guess $\boldsymbol{u}^0_{1\Gamma}$

Calculate $\boldsymbol{u}^0_1 = A^{-1}_{11}(\boldsymbol{f}_1 - A_{1\Gamma}\boldsymbol{u}^0_{1\Gamma})$

Solve for $\boldsymbol{u}^1_2$ and $\boldsymbol{u}^1_{2\Gamma}$, then for $\boldsymbol{u}^2_1$ and $\boldsymbol{u}^2_{1\Gamma}$

Calculate $\boldsymbol{d}^2_{1\Gamma} = \boldsymbol{u}^2_{1\Gamma} - \boldsymbol{u}^0_{1\Gamma}$ and $\boldsymbol{d}^2_1$ and set $n = 2$

while $\|\boldsymbol{d}^n_{1\Gamma}\| + \left\|\boldsymbol{d}^{n-1}_{2\Gamma}\right\| \geq tol$ **do**

    for $i = 1:2$ **do**

        Run an iteration of IAA

        Set $\Delta T^n_{i\to j} = -\boldsymbol{v}^n_i(\boldsymbol{w}^n_i)^\top$

        Solve for $\boldsymbol{d}^{n+1}_{j\Gamma}$ and $\boldsymbol{d}^{n+1}_j$

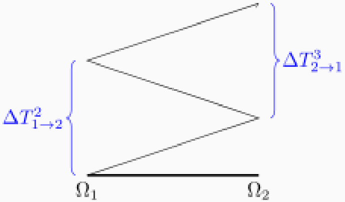
        $\boldsymbol{u}^{n+1}_j := \boldsymbol{u}^{n-1}_j + \boldsymbol{d}^{n+1}_j$, $\boldsymbol{u}^{n+1}_{j\Gamma} := \boldsymbol{u}^{n-1}_{j\Gamma} + \boldsymbol{d}^{n+1}_{j\Gamma}$

        $n \leftarrow n + 1$

    end for

end while

Output: $\boldsymbol{u} = [\boldsymbol{u}^n_1\ ;\ (\boldsymbol{u}^n_{1\Gamma} + \boldsymbol{u}^{n-1}_{2\Gamma})/2\ ;\ \boldsymbol{u}^{n-1}_2]$



$\Delta T^2_{1\to 2}$
$\Delta T^3_{2\to 1}$
Ω_1
Ω_2
$\Delta T^3_{1\to 2}$
$\Delta T^2_{1\to 2}$
$\Delta T^1_{1\to 2}$
$\Delta T^3_{2\to 1}$
$\Delta T^2_{2\to 1}$
$\Delta T^1_{2\to 1}$
Ω_1
Ω_2

AOSM Galerkin condition

Theorem

If $\hat{A} + E_{i\to j}^{n+1}$ is invertible, then the update to the solution due to an AOSM is

$$\boldsymbol{d}_{j\Gamma}^{n+1} = \left(\hat{A} + E_{i\to j}^{n}\right)^{-1} E_{i\to j}^{n} \boldsymbol{x},$$

where $\boldsymbol{x} \in \operatorname{span}(W_i^n)$ such that the residual of

$$\left(I - \left(\hat{A} + E_{i\to j}^{n+1}\right)^{-1} E_{i\to j}^{n+1}\right) \boldsymbol{u}_\Gamma$$
$$= \left(\hat{A} + E_{i\to j}^{n+1}\right)^{-1} \left(\boldsymbol{f}_\Gamma - A_{\Gamma j} A_{jj}^{-1} \boldsymbol{f}_j - A_{\Gamma i} A_{ii}^{-1} \boldsymbol{f}_i\right)$$

applied to $\boldsymbol{u}_{i\Gamma}^{n-1} + \boldsymbol{x}$ is orthogonal to $\operatorname{span}(W_i^n)$.

Numerical results

$$\begin{cases} \Delta u(x,y) = f(x,y), & (x,y) \in \Omega = [-1,1] \times [-1,1], \\ u(x,y) = g(x,y), & (x,y) \in \partial\Omega. \end{cases}$$

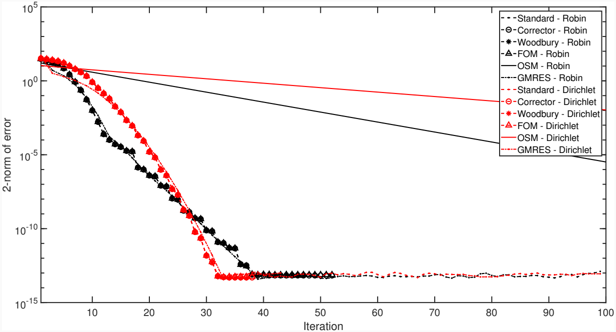


Figure 1: Comparison of altAOSM versions with $N = 10,000$, $M = 100$, using both Robin and Dirichlet boundary conditions.

Conclusions and Future Work

- AOSMs give convergence rates comparable to Krylov subspace methods, but without the extra computations.
- Transmission conditions from AOSMs can be re-used to give fast convergence when repeated solves are required.
- Nested decompositions will allow more subdomains, but crosspoints need to be resolved for more general decompositions.