A posteriori error estimation for overlapping Schwarz solvers

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1. Adjoint-based error estimation

We wish to solve the linear system of equations

$$Au = f \tag{1}$$

and determine a linear functional of solution u, namely the "quantity of interest"

$$Q = (\psi, u). \tag{2}$$

Assume that we have an approximate solution $\hat{u} \approx u$, such that

$$A\hat{u} = \hat{f}. \tag{3}$$

The error in the quantity of interest Q is

$$(\psi, u) - (\psi, \hat{u}) = (\psi, u - \hat{u}) = (\psi, e), \tag{4}$$

where $e = u - \hat{u}$.

In order to construct a *computable* estimate for the error in the QoI, we define and solve the *adjoint* equation

$$A^{\top}\phi = \psi, \tag{5}$$

for adjoint solution ϕ, and observe that

$$(\psi, e) = (A^{\top}\phi, e) = (\phi, Ae) = (\phi, A(u - \hat{u})) = (\phi, f - \hat{f}) = (\phi, r), \tag{6}$$

where the *residual* $r = f - \hat{f}$.

2. Iterative solvers for linear systems

We wish to solve the linear system of equations

$$Au = f.$$

Assuming it is not possible to invert A directly, we seek to compute an approximation $\bar{u}$ to solution u via an iterative procedure. Let $\bar{u}$ be an approximation to u, such that

$$A\bar{u} = \bar{f}. \tag{7}$$

We seek to iteratively improve this approximation. Formally,

$$u - \bar{u} = A^{-1}f - A^{-1}\bar{f} = A^{-1}r$$

where again the *residual* $r = f - \bar{f}$.

Let B be any approximation to A^{-1} and construct the iteration: Given $u^{\{0\}}$, find

$$\begin{aligned} u^{\{k\}} &= u^{\{k-1\}} + Br = u^{\{k-1\}} + B\left(f - Au^{\{k-1\}}\right), \quad k = 1, 2, \ldots, \\ &= (I - BA)u^{\{k-1\}} + Bf, \quad k = 0, 1, \ldots. \end{aligned} \tag{8}$$

Let $u^{\{k\}}$ be the analytic or exact solution to an iterative procedure, and $\hat{u}^{\{k\}}$ be an approximation to $u^{\{k\}}$. We partition the total error into the error arising due to the iterative process, and the error due to the inexact solution of the iterative equations, i.e.,

$$\begin{aligned} \text{Total error, } e^{\{k\}} &= u - \hat{u}^{\{k\}} \\ &= (u - u^{\{k\}}) + (u^{\{k\}} - \hat{u}^{\{k\}}) \\ &= \text{Iteration error} + \text{Discretization error}. \end{aligned} \tag{9}$$

The total error in the QoI can be partitioned similarly, i.e.,

$$\begin{aligned} \text{Total error in QoI, } (e^{\{k\}}, \psi) &= (u - \hat{u}^{\{k\}}, \psi) \\ &= (u - u^{\{k\}}, \psi) + (u^{\{k\}} - \hat{u}^{\{k\}}, \psi) \\ &= \text{Iteration error in QoI} + \text{Discretization error in QoI}. \end{aligned} \tag{10}$$

We will compute the iteration error as the difference between the total and discretization errors.

Remark 1. *We require the spectral radius of $(I - BA)$ to be less than one to ensure convergence. See [1, 2, 3] for details of the convergence of additive and restricted additive Schwarz methods.*

3. Overlapping Schwarz iterative solvers

We wish to solve the linear system of equation

$$Au = f$$

where $A \in \mathbb{R}^{n\times n}$, $u \in \mathbb{R}^n$ and $f \in \mathbb{R}^n$ by an overlapping Schwarz method and estimate the error in a quantity of interest

$$\text{QoI} = (\psi, u)\,,$$

where $\psi \in \mathbb{R}^n$.

Index set $\mathcal{I}$: Let $\mathcal{I}$ be the index set

$$\mathcal{I} = \{1, 2, \cdots, n\}.$$

Overlapping decomposition of $\mathcal{I}$: We construct an overlapping decomposition of the index set $\mathcal{I}$ given by $\mathcal{I}_i, i = 1, 2, \ldots, p$ such that

$$\cup_{i=1}^{p} \mathcal{I}_i = \mathcal{I}$$

where $|\mathcal{I}_i| = m_i$ and $\sum_{i=1}^{p} m_i > n$.

Subdomain restriction operators: We define the subdomain *restriction* operators (matrices) R_i,

$$R_i \in \mathbb{R}^{m_i \times n},\ i = 1, 2, \ldots, p,$$

to be rank m_i matrices with rows $e_j^\top$ for $j \in \mathcal{I}_i$, where $e_j \in \mathbb{R}^n$ is a vector of zeros with a single one in column j.

Partition of $\mathcal{I}$: Construct an non-overlapping partition of the index set $\mathcal{P}$ given by $\mathcal{P}_i, i = 1, 2, \ldots, p$ such that

$$\cup_{i=1}^{p} \mathcal{P}_i = \mathcal{I}$$

and

$$\mathcal{P}_i \cap \mathcal{P}_j = \phi,\ \text{for all } i \neq j,$$

where $|\mathcal{P}_i| = q_i$ and $\sum_{i=1}^{p} q_i = n$.

Partition restriction operators: We define the partition *restriction* operators (matrices) $\widetilde{R}_i$,

$$\widetilde{R}_i \in \mathbb{R}^{m_i \times n},\ i = 1, 2, \ldots, p,$$

to be rank q_i matrices with rows $e_j^\top$ for $j \in \mathcal{I}_i \cap \mathcal{P}_i$. The partition restriction operator $\widetilde{R}_i$ is constructed from the subdomain restriction operator R_i by removing the single one (in column j) in the rows of R_i for which $j \in \mathcal{I}_i$, but $j \notin \mathcal{P}_i$.

4. Additive Schwarz

4.1. Forward problem

We define

$$\begin{aligned}A_i &= R_i A R_i^\top, \in \mathbb{R}^{m_i \times m_i},\ i = 1, 2, \ldots, p,\\ B_i &= R_i^\top A_i^{-1} R_i = R_i^\top \left(R_i A R_i^\top\right)^{-1} R_i \in \mathbb{R}^{n\times n},\ i = 1, 2, \ldots, p,\\ C_i &= B_i A \in \mathbb{R}^{n\times n},\ i = 1, 2, \ldots, p,\\ f_i &= B_i f \in \mathbb{R}^n,\ i = 1, 2, \ldots, p.\end{aligned} \tag{11}$$

Single iteration: The additive Schwarz algorithm is: Given $u^{\{0\}}$ and $\alpha < 1$, for $k = 1, 2, \ldots$

$$\begin{aligned}u^{\{k\}} &= u^{\{k-1\}} + \alpha \sum_{i=1}^{p} B_i \left(f - A u^{\{k-1\}}\right),\\ &= \left(I - \alpha \sum_{i=1}^{p} B_i A\right) u^{\{k-1\}} + \alpha \sum_{i=1}^{p} B_i f\\ &= \left(I - \alpha \sum_{i=1}^{p} C_i\right) u^{\{k-1\}} + \alpha \sum_{i=1}^{p} f_i\\ &= D u^{\{k-1\}} + g,\end{aligned} \tag{12}$$

where

$$D = I - \alpha \sum_{i=1}^{p} C_i \quad \text{and} \quad g = \alpha \sum_{i=1}^{p} f_i. \tag{13}$$

Note that relaxation is required and the p subdomain components, each of which is of size n, can be solved in parallel.

K iterations: Using this notation and assuming $u^{\{0\}} = 0$, $K = 6$ iterations of additive Schwarz can be written as the nK dimensional system of equations

$$U = \begin{bmatrix} I & 0 & 0 & 0 & 0 & 0\\ -D & I & 0 & 0 & 0 & 0\\ 0 & -D & I & 0 & 0 & 0\\ 0 & 0 & -D & I & 0 & 0\\ 0 & 0 & 0 & -D & I & 0\\ 0 & 0 & 0 & 0 & -D & I \end{bmatrix} \begin{pmatrix} u^{\{1\}}\\ u^{\{2\}}\\ u^{\{3\}}\\ u^{\{4\}}\\ u^{\{5\}}\\ u^{\{6\}} \end{pmatrix} = \begin{pmatrix} g\\ g\\ g\\ g\\ g\\ g \end{pmatrix}. \tag{14}$$

This system nK linear equations can be solved (blockwise) by forward substitution.

4.2. Adjoint equations

The adjoint system of equations of size nK to (14), for the error in the QoI $(\psi, u^{\{K\}} - \hat{u}^{\{K\}})$ is

$$U^\top x = \begin{bmatrix} I & -D^\top & 0 & 0 & 0 \\ 0 & I & -D^\top & 0 & 0 \\ 0 & 0 & I & -D^\top & 0 \\ 0 & 0 & 0 & I & -D^\top \\ 0 & 0 & 0 & 0 & I \end{bmatrix} \begin{pmatrix} \phi^{\{1\}}\\ \phi^{\{2\}}\\ \phi^{\{3\}}\\ \phi^{\{4\}}\\ \phi^{\{5\}}\\ \phi^{\{6\}} \end{pmatrix} = \begin{pmatrix} 0\\ 0\\ 0\\ 0\\ 0\\ \psi \end{pmatrix},$$

where $\psi \in \mathbb{R}^n$. This system nK linear equations can be solved (blockwise) by backward substitution. Finally, note that

$$\begin{aligned} \phi^{\{K\}} &= \psi \\ \phi^{\{K-1\}} &= D^\top \phi^{\{K\}} = D^\top \psi \\ &\vdots \\ \phi^{\{1\}} &= \underbrace{D^\top \dots D^\top}_{K \text{ times}} \psi. \end{aligned} \tag{15}$$

4.3. Discretization error representation

The discretization error in the QoI defined in (10) is given by the inner product

$$\text{Discretization error in QoI} = (\psi, u^{\{K\}} - \hat{u}^{\{K\}}) = (R, \Phi), \tag{16}$$

where R is nK-dimensional vector of residuals and

$$\Phi = \begin{pmatrix} \phi^{\{1\}} \\ \phi^{\{2\}} \\ \vdots \\ \phi^{\{K\}} \end{pmatrix}. \tag{17}$$

4.4. Total error representation

Assuming the global adjoint problem (5) can be solved for global adjoint solution ϕ, i.e., solving (5)

$$A^\top \phi = \psi,$$

and defining residual

$$r = f - A\hat{u}^{\{K\}}, \tag{18}$$

then

$$\text{Total error in QoI} = (r, \phi) \tag{19}$$

and

$$\text{Iterative error in QoI} = \text{Total error in QoI} - \text{Discretization error in QoI}. \tag{20}$$

4.5. Error accumulation

We assume that an error is made at each subdomain solve. Let $\varepsilon \in \mathbb{R}^{npK}$ be a random vector representing numerical errors and $\mu^{\{k,i\}} \in \mathbb{R}^n$ be the components of the vector ε from $(k-1)np + (i-1)n + 1$ to $(k-1)np + in$. Then, let

$$u^{\{k\}} = u^{\{k-1\}} + \alpha \left(\sum_{i=1}^{p} B_i \left(f - Au^{\{k-1\}} \right) + \mu^{\{k,i\}} \right). \tag{21}$$

The error made each iteration ("sweep") of additive Schwarz is

$$\epsilon^{\{k\}} = \sum_{i=1}^{p} \alpha \mu^{\{k,i\}}. \tag{22}$$

In particular,

$$\hat{u}^{\{1\}} = g + \epsilon^{\{1\}} = u^{\{1\}} + \epsilon^{\{1\}}, \tag{23}$$

and

$$\begin{aligned}\hat{u}^{\{2\}} &= g + D\hat{u}^{\{1\}} + \epsilon^{\{2\}} \\ &= g + D\left(g + \epsilon^{\{1\}}\right) + \epsilon^{\{2\}} \\ &= g + Dg + D\epsilon^{\{1\}} + \epsilon^{\{2\}} \\ &= u^{\{2\}} + D\epsilon^{\{1\}} + \epsilon^{\{2\}} \\ &\neq u^{\{2\}} + \epsilon^{\{2\}},\end{aligned} \tag{24}$$

and

$$\begin{aligned}\hat{u}^{\{3\}} &= g + D\hat{u}^{\{2\}} + \epsilon^{\{3\}} \\ &= g + D\left(g + Dg + D\epsilon^{\{1\}} + \epsilon^{\{2\}}\right) + \epsilon^{\{3\}} \\ &= g + Dg + D^2g + D^2\epsilon^{\{1\}} + D\epsilon^{\{2\}} + \epsilon^{\{3\}} \\ &= u^{\{3\}} + D^2\epsilon^{\{1\}} + D\epsilon^{\{2\}} + \epsilon^{\{3\}} \\ &\neq u^{\{3\}} + \epsilon^{\{3\}}.\end{aligned} \tag{25}$$

Continuing,

$$\begin{aligned}\hat{u}^{\{K\}} &= u^{\{K\}} + \sum_{i=1}^{K} D^{K-i}\epsilon^{\{i\}} \\ &\neq u^{\{K\}} + \epsilon^{\{K\}}\end{aligned} \tag{26}$$

This *accumulation of error* must be recognized if the same vector $\varepsilon \in \mathbb{R}^{npK}$ is used when solving a sequence of K single iterations of the form (12) and when solving K iterations as a single linear system of the form (14). This is accomplished in the codes by setting the logical variable `accum` to be true.

5. Restricted Additive Schwarz

5.1. Forward problem

We define

$$\begin{aligned}
A_i &= R_i A R_i^\top, \in \mathbb{R}^{m_i \times m_i},\ i = 1, 2, \ldots, p, \\
\widetilde{B}_i &= \widetilde{R}_i^\top A_i^{-1} R_i = \widetilde{R}_i^\top \left(R_i A R_i^\top\right)^{-1} R_i \in \mathbb{R}^{n \times n},\ i = 1, 2, \ldots, p, \\
\widetilde{C}_i &= \widetilde{B}_i A \in \mathbb{R}^{n \times n},\ i = 1, 2, \ldots, p, \\
\widetilde{f}_i &= \widetilde{B}_i f \in \mathbb{R}^n,\ i = 1, 2, \ldots, p.
\end{aligned} \tag{27}$$

<u>Single iteration:</u> The additive Schwarz algorithm is: For $k = 0, 1, \ldots$

$$\begin{aligned}
u^{\{k\}} &= u^{\{k-1\}} + \sum_{i=1}^{p} \widetilde{B}_i \left(f - A u^{\{k-1\}}\right), \\
&= \left(I - \sum_{i=1}^{p} \widetilde{B}_i A\right) u^{\{k-1\}} + \sum_{i=1}^{p} \widetilde{B}_i f \\
&= (I - \widetilde{C}) u^{\{k-1\}} + \sum_{i=1}^{p} \widetilde{f}_i \\
&= \widetilde{D} u^{\{k-1\}} + \widetilde{g}
\end{aligned} \tag{28}$$

where

$$\widetilde{C} = \sum_{i=1}^{p} \widetilde{C}_i, \quad \widetilde{D} = I - \widetilde{C} \text{ and } \widetilde{g} = \sum_{i=1}^{p} \widetilde{f}. \tag{29}$$

Note that *no* relaxation is required and the p subdomain components, each of which is of size n, can be solved in parallel.

<u>K iterations:</u> Using this notation and assuming $u^{\{0\}} = 0$, $K = 6$ iterations of restricted additive Schwarz can be written as the nK dimensional system of equations

$$U = \begin{bmatrix} I & 0 & 0 & 0 & 0 & 0 \\ -\widetilde{D} & I & 0 & 0 & 0 & 0 \\ 0 & -\widetilde{D} & I & 0 & 0 & 0 \\ 0 & 0 & -\widetilde{D} & I & 0 & 0 \\ 0 & 0 & 0 & -\widetilde{D} & I & 0 \\ 0 & 0 & 0 & 0 & -\widetilde{D} & I \end{bmatrix} \begin{pmatrix} u^{\{1\}} \\ u^{\{2\}} \\ u^{\{3\}} \\ u^{\{4\}} \\ u^{\{5\}} \\ u^{\{6\}} \end{pmatrix} = \begin{pmatrix} \widetilde{g} \\ \widetilde{g} \\ \widetilde{g} \\ \widetilde{g} \\ \widetilde{g} \\ \widetilde{g} \end{pmatrix}. \tag{30}$$

This system nK linear equations can be solved (blockwise) by forward substitution.

5.2. Adjoint equations

The adjoint system of equations of size nK to (30), for the error in the QoI $(\psi, u^{\{K\}} - \hat{u}^{\{K\}})$ is

$$U^\top x = \begin{bmatrix} I & -\widetilde{D}^\top & 0 & 0 & 0 \\ 0 & I & -\widetilde{D}^\top & 0 & 0 \\ 0 & 0 & I & -\widetilde{D}^\top & 0 \\ 0 & 0 & 0 & I & -\widetilde{D}^\top \\ 0 & 0 & 0 & 0 & I \end{bmatrix} \begin{pmatrix} \phi^{\{1\}} \\ \phi^{\{2\}} \\ \phi^{\{3\}} \\ \phi^{\{4\}} \\ \phi^{\{5\}} \\ \phi^{\{6\}} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \psi \end{pmatrix},$$

where $\psi \in \mathbb{R}^n$. This system nK linear equations can be solved (blockwise) by backward substitution. Finally, note that

$$
\begin{aligned}
\phi^{\{K\}} &= \psi \\
\phi^{\{K-1\}} &= \widetilde{D}^\top \phi^{\{K\}} = \widetilde{D}^\top \psi \\
&\vdots \\
\phi^{\{1\}} &= \underbrace{\widetilde{D}^\top \ldots \widetilde{D}^\top}_{K \text{ times}} \psi.
\end{aligned}
$$

5.3. *Discretization error representation*

The error in the QoI defined by (10) is given by the inner product

$$\text{Discretization error} = (\psi, u^{\{K\}} - \hat{u}^{\{K\}}) = (R, \Phi),$$

where R is nK-dimensional vector of residuals and

$$\Phi = \begin{pmatrix} \phi^{\{1\}} \\ \phi^{\{2\}} \\ \vdots \\ \phi^{\{K\}} \end{pmatrix}.$$

5.4. *Total error representation*

The total error and iterative error are computed as in §4.4.

6. Multiplicative Schwarz

The notation for multiplicative Schwarz becomes more complicated if every global solution is stored. There are p such global solutions per "sweep" and pK such solutions for K sweeps of multiplicative Schwarz.

$$
\begin{aligned}
&u \in \mathbb{R}^n, v \in \mathbb{R}^{np}, w \in \mathbb{R}^{npK},\\
&f \in \mathbb{R}^n, g \in \mathbb{R}^{np}, h \in \mathbb{R}^{npK},\\
&\phi \in \mathbb{R}^n, \Phi \in \mathbb{R}^{np}, \Theta \in \mathbb{R}^{npK},\\
&\psi \in \mathbb{R}^n, \Psi \in \mathbb{R}^{np}, \Xi \in \mathbb{R}^{npK}.
\end{aligned}
$$

6.1. Forward problem

We define

$$
\begin{aligned}
A_i &= R_i A R_i^\top, \in \mathbb{R}^{m_i \times m_i},\ i = 1, 2, \dots, p,\\
B_i &= R_i^\top A_i^{-1} R_i = R_i^\top \left(R_i A R_i^\top\right)^{-1} R_i \in \mathbb{R}^{n \times n},\ i = 1, 2, \dots, p,\\
C_i &= B_i A \in \mathbb{R}^{n \times n},\ i = 1, 2, \dots, p,\\
D_i &= (I - C_i) \in \mathbb{R}^{n \times n},\ i = 1, 2, \dots, p,\\
f_i &= B_i f \in \mathbb{R}^n,\ i = 1, 2, \dots, p.
\end{aligned}
\tag{31}
$$

Single iteration: The multiplicative Schwarz algorithm is: Given $u^{\{0\}}$, for $k = 0, 1, \dots$

$$
\begin{aligned}
u^{\{k+i/p\}} &= u^{\{k+(i-1)/p\}} + B_i \left(f - A u^{\{k+(i-1)/p\}}\right),\ i = 1, 2, \dots, p,\\
&= (I - B_i A) u^{\{k+(i-1)/p\}} + B_i f\\
&= (I - C_i) u^{\{k+(i-1)/p\}} + B_i f\\
&= D_i u^{\{k+(i-1)/p\}} + f_i
\end{aligned}
\tag{32}
$$

Assume $p = 5$ and let

$$
\begin{aligned}
S &= \begin{bmatrix} I & 0 & 0 & 0 & 0 \\ -D_2 & I & 0 & 0 & 0 \\ 0 & -D_3 & I & 0 & 0 \\ 0 & 0 & -D_4 & I & 0 \\ 0 & 0 & 0 & -D_5 & I \end{bmatrix} \in \mathbb{R}^{np \times np}, \\
T &= \begin{bmatrix} 0 & 0 & 0 & 0 & -D_1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix} \in \mathbb{R}^{np \times np}, \\
g &= \begin{pmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \end{pmatrix} \in \mathbb{R}^{np}, \\
v^{\{k\}} &= \begin{pmatrix} u^{\{(k-1)+1/5\}} \\ u^{\{(k-1)+2/5\}} \\ u^{\{(k-1)+3/5\}} \\ u^{\{(k-1)+4/5\}} \\ u^{\{k\}} \end{pmatrix} \in \mathbb{R}^{np},
\end{aligned}
\tag{33}
$$

then, defining

$$
v^{\{0\}} = \begin{pmatrix} 0 \\ \vdots 0 \\ u^{\{0\}} \end{pmatrix},
$$

a single “sweep” of multiplicative Schwarz can be written as

$$
Sv^{\{k\}} + Tv^{\{k-1\}} = g, \quad k = 1, 2, \ldots. \tag{34}
$$

<u>K iterations:</u> Assuming $u^{\{0\}} = 0$ and therefore $v^{\{0\}} = 0$, $K = 6$ iterations of multiplicative Schwarz can be written as the npK dimensional system of equations

$$
\begin{bmatrix} S & 0 & 0 & 0 & 0 & 0 \\ T & S & 0 & 0 & 0 & 0 \\ 0 & T & S & 0 & 0 & 0 \\ 0 & 0 & T & S & 0 & 0 \\ 0 & 0 & 0 & T & S & 0 \\ 0 & 0 & 0 & 0 & T & S \end{bmatrix} \begin{pmatrix} v^{\{1\}} \\ v^{\{2\}} \\ v^{\{3\}} \\ v^{\{4\}} \\ v^{\{5\}} \\ v^{\{6\}} \end{pmatrix} = \begin{pmatrix} g \\ g \\ g \\ g \\ g \\ g \end{pmatrix}. \tag{35}
$$

This system npK linear equations can be solved (np-blockwise) by forward substitution. Furthermore, each np-dimensional block can be solved by (n-blockwise) forward substitution.

Now write (35) as the npK-dimensional system

$$
Uw = h, \tag{36}
$$

where

$$
U = \begin{bmatrix} S & 0 & 0 & 0 & 0 & 0 \\ T & S & 0 & 0 & 0 & 0 \\ 0 & T & S & 0 & 0 & 0 \\ 0 & 0 & T & S & 0 & 0 \\ 0 & 0 & 0 & T & S & 0 \\ 0 & 0 & 0 & 0 & T & S \end{bmatrix} \in \mathbb{R}^{npK \times npK},
$$

$$
w = \begin{pmatrix} v^{\{1\}} \\ v^{\{2\}} \\ v^{\{3\}} \\ v^{\{4\}} \\ v^{\{5\}} \\ v^{\{6\}} \end{pmatrix} \in \mathbb{R}^{npK}, \tag{37}
$$

$$
h = \begin{pmatrix} g \\ g \\ g \\ g \\ g \\ g \end{pmatrix} \in \mathbb{R}^{npK}.
$$

6.2. Adjoint equations

The adjoint system of equations to (35), for the error in the QoI $(\psi, u^{\{K\}} - \hat{u}^{\{K\}})$, can be constructed in a straightforward manner by defining

$$
S^\top = \begin{bmatrix} I & -D_2^\top & 0 & 0 & 0 \\ 0 & I & -D_3^\top & 0 & 0 \\ 0 & 0 & I & -D_4^\top & 0 \\ 0 & 0 & 0 & I & -D_5^\top \\ 0 & 0 & 0 & 0 & I \end{bmatrix},
$$

$$
\text{and} \quad T^\top = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ -D_1^\top & 0 & 0 & 0 & 0 \end{bmatrix}.
$$

The adjoint system of size npK is

$$
\begin{bmatrix} S^\top & T^\top & 0 & 0 & 0 & 0 \\ 0 & S^\top & T^\top & 0 & 0 & 0 \\ 0 & 0 & S^\top & T^\top & 0 & 0 \\ 0 & 0 & 0 & S^\top & T^\top & 0 \\ 0 & 0 & 0 & 0 & S^\top & T^\top \\ 0 & 0 & 0 & 0 & 0 & S^\top \end{bmatrix} \begin{pmatrix} \Phi^{\{1\}} \\ \Phi^{\{2\}} \\ \Phi^{\{3\}} \\ \Phi^{\{4\}} \\ \Phi^{\{5\}} \\ \Phi^{\{6\}} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \Psi \end{pmatrix},
$$

where $\Phi^{\{k\}} \in \mathbb{R}^{np}, k = 1, 2, \cdots, K$. Here

$$\Phi^{\{k\}} = \begin{pmatrix} \phi^{\{(k-1)+1/5\}} \\ \phi^{\{(k-1)+2/5\}} \\ \phi^{\{(k-1)+3/5\}} \\ \phi^{\{(k-1)+4/5\}} \\ \phi^{\{k\}} \end{pmatrix},$$

where $\phi^{\{(k-1)+i/p\}} \in \mathbb{R}^n$, and

$$\Psi = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \psi \end{pmatrix},$$

$\Psi \in \mathbb{R}^{np}$, where $\psi \in \mathbb{R}^n$.

This system npK linear equations can be solved (blockwise) by backward substitution. Furthermore, the np-dimensional systems of equations within each block can be solved by backward substitution. This is particularly simple due to the identity matrices on the diagonal of S and therefore of $S^\top$. Solving the adjoint system,

$$\begin{aligned} \phi^{\{K\}} &= \psi \\ \phi^{\{K-1+(p-1)/p\}} &= D_p^\top \psi \\ \phi^{\{K-1+(p-2)/p\}} &= D_{p-1}^\top D_p^\top \psi \\ &\vdots \\ \phi^{\{K-1+1/p\}} &= D_2^\top \cdots D_{p-1}^\top D_p^\top \psi = E^\top \psi \\ \phi^{\{K-1\}} &= D_1^\top D_2^\top \cdots D_{p-1}^\top D_p^\top \psi = D_1^\top E^\top \psi \\ &\vdots \\ \phi^{\{1/p\}} &= E^\top \underbrace{\left(D_1^\top E^\top\right)\left(D_1^\top E^\top\right) \cdots \left(D_1^\top E^\top\right)}_{K-1 \text{ times}} \psi \end{aligned} \tag{38}$$

where we have defined $E^\top = D_2^\top \cdots D_{p-1}^\top D_p^\top$.

We write this compactly as

$$U^\top \Theta = \Xi, \tag{39}$$

where

$$
\begin{aligned}
\Theta &= \begin{pmatrix} \Phi^{\{1\}} \\ \Phi^{\{2\}} \\ \Phi^{\{3\}} \\ \Phi^{\{4\}} \\ \Phi^{\{5\}} \\ \Phi^{\{6\}} \end{pmatrix} \in \mathbb{R}^{npK}, \\
\Xi &= \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \Psi \end{pmatrix} \in \mathbb{R}^{npK}.
\end{aligned} \tag{40}
$$

6.3. Discretization error representation

The discretization error in the QoI defined by (10) is given by the inner product

$$
\text{Discretization error} = (u^{\{K\}} - \hat{u}^{\{K\}}, \psi) = (R, \Theta),
$$

where R is npK-dimensional vector of residuals and

$$
\Theta = \begin{pmatrix} \Phi^{\{1\}} \\ \Phi^{\{2\}} \\ \vdots \\ \Phi^{\{K\}} \end{pmatrix}.
$$

6.4. Total error representation

The total error and iterative error are computed as in §4.4.

6.5. Error accumulation

We assume that an error is made at each subdomain solve. Let $\varepsilon \in \mathbb{R}^{npK}$ be a random vector representing numerical errors and $\epsilon^{\{i\}} \in \mathbb{R}^n$ be the components of the vector ε from $(k-1)np + (i-1)n + 1$ to $(k-1)np + in$. Then, let

$$
u^{\{k+i/p\}} = D_i u^{\{k-(i-1)/p\}} + f_i. \tag{41}
$$

In particular, if $u^{\{0\}} = 0$

$$
\hat{u}^{\{1/p\}} = f_1 + \epsilon^{\{1\}} = u^{\{1/p\}} + \epsilon^{\{1\}}, \tag{42}
$$

and

$$
\begin{aligned}
\hat{u}^{\{2/p\}} &= D_2 \hat{u}^{\{1/p\}} + f_2 + \epsilon^{\{2\}} \\
&= D_2 (f_1 + \epsilon^{\{1\}}) + f_2 + \epsilon^{\{2\}} \\
&= (D_2 f_1 + f_2) + D_2 \epsilon^{\{1\}} + \epsilon^{\{2\}} \\
&= u^{\{2/p\}} + D_2 \epsilon^{\{1\}} + \epsilon^{\{2\}} \\
&\neq u^{\{2/p\}} + \epsilon^{\{2\}},
\end{aligned} \tag{43}
$$

and

$$
\begin{aligned}
\hat{u}^{\{3/p\}} &= D_3 \hat{u}^{\{2/p\}} + f_3 + \epsilon^{\{3\}} \\
&= D_3((D_2 f_1 + f_2) + (D_2 \epsilon^{\{1\}} + \epsilon^{\{2\}})) + \epsilon^{\{3\}} \\
&= D_3(D_2 f_1 + f_2) + D_3(D_2 \epsilon^{\{1\}} + \epsilon^{\{2\}}) + \epsilon^{\{3\}} \\
&= u^{\{3/p\}} + D_3(D_2 \epsilon^{\{1\}} + \epsilon^{\{2\}}) + \epsilon^{\{3\}} \\
&\neq u^{\{3/p\}} + \epsilon^{\{3\}}.
\end{aligned}
\tag{44}
$$

Clearly at iteration $(k+i/p)$ is D_i times the error at iteration $(k+(i-1)/p)$ plus the "new" error at iteration $(k+i/p)$. This *accumulation of error* must be recognized if the same vector $\varepsilon \in \mathbb{R}^{npK}$ is used when solving a sequence of pK single iterations of the form (32) and when solving K iterations as a single linear system of the form (36). This is accomplished in the codes by setting the logical variable `accum` to be true.

7. Results

7.1. Additive Schwarz

Here mpert is the variance of the normally distributed mean zero numerical error added to each solve and ν is the effectivity ratio of the adjoint-based *a posteriori* error estimator

K	α	mpert	Discretization error	ν	Total error	ν	Iterative error
12	0.01	1.0e-02	-1.11e-03	1.0	5.13e-01	1.0	5.14e-01
12	0.10	1.0e-02	1.93e-03	1.0	5.61e-01	1.0	5.59e-01
12	0.25	1.0e-02	1.71e-02	1.0	2.21e-01	1.0	2.03e-01
12	0.50	1.0e-02	3.12e-02	1.0	5.31e-02	1.0	2.19e-02
12	0.75	1.0e-02	1.40e-02	1.0	7.40e-02	1.0	6.00e-02
12	0.90	1.0e-02	-1.30e+00	1.0	1.91e+00	1.0	3.21e+00
12	0.99	1.0e-02	-7.74e+00	1.0	1.33e+01	1.0	2.10e+01

Table 1: Additive Schwarz: Effect of α

K	α	mpert	Discretization error	ν	Total error	ν	Iterative error
24	0.5	1.0E-01	-6.37E-01	1.0	-6.36E-01	1.0	3.70E-04
24	0.5	1.0E-02	-6.37E-02	1.0	-6.33E-02	1.0	3.70E-04
24	0.5	1.0E-03	-6.37E-03	1.0	-6.00E-03	1.0	3.70E-04
24	0.5	1.0E-04	-6.37E-04	1.0	-2.67E-04	1.0	3.70E-04
24	0.5	1.0E-05	-6.37E-05	1.0	3.06E-04	1.0	3.70E-04

Table 2: Additive Schwarz: Effect of mpert

K	α	mpert	Discretization error	ν	Total error	ν	Iterative error
3	0.5	1.00E-03	2.47E-04	1.0	4.79E-01	1.0	4.79E-01
6	0.5	1.00E-03	1.21E-03	1.0	1.72E-01	1.0	1.71E-01
12	0.5	1.00E-03	3.12E-03	1.0	2.50E-02	1.0	2.19E-02
24	0.5	1.00E-03	-6.37E-03	1.0	-6.00E-03	1.0	3.70E-04
48	0.5	1.00E-03	-7.15E-04	1.0	-7.15E-04	1.0	1.04E-07

Table 3: Additive Schwarz: Effect of K

7.2. Restricted Additive Schwarz

K	mpert	Discretization error	ν	Total error	ν	Iterative error
24	1.0E-02	-1.33E-01	1.0	-1.33E-01	1.0	1.39E-06
24	1.0E-04	-1.33E-03	1.0	-1.33E-03	1.0	1.39E-06
24	1.0E-06	-1.33E-05	1.0	-1.19E-05	1.0	1.39E-06
24	1.0E-08	-1.33E-07	1.0	1.26E-06	1.0	1.39E-06

Table 4: Restricted Additive Schwarz: Effect of mpert

K	mpert	Discretization error	ν	Total error	ν	Iterative error
3	1.00E-03	6.67E-04	1.0	2.04E-01	1.0	2.03E-01
6	1.00E-03	6.05E-03	1.0	3.96E-02	1.0	3.35E-02
12	1.00E-03	2.95E-03	1.0	4.06E-03	1.0	1.11E-03
24	1.00E-03	-1.33E-02	1.0	-1.33E-02	1.0	1.39E-06
48	1.00E-03	6.89E-04	1.0	6.89E-04	1.0	2.14E-12

Table 5: Restricted Additive Schwarz: Effect of K

7.3. Multiplicative Schwarz

K	mpert	Discretization error	ν	Total error	ν	Iterative error
6	1.00E-02	1.30E-01	1.0	1.31E-01	1.0	5.94E-04
6	1.00E-03	1.30E-02	1.0	1.36E-02	1.0	5.94E-04
6	1.00E-04	1.30E-03	1.0	1.90E-03	1.0	5.94E-04
6	1.00E-05	1.30E-04	1.0	7.25E-04	1.0	5.94E-04
6	1.00E-06	1.30E-05	1.0	6.07E-04	1.0	5.94E-04
6	1.00E-08	1.30E-07	1.0	5.95E-04	1.0	5.94E-04

Table 6: Multiplicative Schwarz: Effect of mpert

K	mpert	Discretization error	ν	Total error	ν	Iterative error
3	1.00E-04	-4.83E-04	1.0	4.15E-02	1.0	4.20E-02
6	1.00E-04	1.30E-03	1.0	1.90E-03	1.0	5.94E-04
12	1.00E-04	3.04E-04	1.0	3.04E-04	1.0	1.15E-07
24	1.00E-04	-3.22E-05	1.0	-3.22E-05	1.0	4.08E-15

Table 7: Multiplicative Schwarz: Effect of K

7.4. Running the codes

The results presented above can be obtained from the Matlab code using the system and error vector stored in ....

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List of Tables