A posteriori error analysis for Schwarz overlapping domain decomposition methods

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Abstract

Domain decomposition methods are widely used for the numerical solution of partial differential equations on parallel computers. We develop an adjoint-based a posteriori error analysis for overlapping multiplicative Schwarz and for overlapping additive Schwarz domain decomposition methods. In both cases the numerical error in a user-specified functional of the solution (quantity of interest), is decomposed into a component that arises as a result of the finite iteration between the subdomains, and a component that is due to the spatial discretization. The spatial discretization error can be further decomposed into the errors arising on each subdomain. This decomposition of the total error can then be used as part of a two-stage approach to construct a solution strategy that efficiently reduces the error in the quantity of interest.

1 Introduction

We derive and implement an adjoint-based a posteriori error analysis for overlapping domain decomposition methods for boundary value problems, examining both additive and multiplicative Schwarz algorithms. Domain decomposition methods (DDMs) arrive at the solution of a problem defined over a domain by combining the solutions of related problems posed on subdomains. The problems posed on subdomains often require less computational resources and some of the first uses of DDMs for practical applications were in low-memory or limited computation scenarios [24, 29]. Recently DDMs have seen increased use in the context of distributed and parallel computing. There are a number of excellent references for the theory and implementation of DDMs [32, 34, 33, 28, 23]. In this article we follow the presentation in [28].

In overlapping DDMs, each subdomain has a non-empty intersection with at least one other subdomain and typically only state information is exchanged between the subdomains. The theoretical properties of the multiplicative Schwarz method and some of its variants were studied in [25]. The variant of this method suitable for parallel computing, called the additive Schwarz method, was introduced in [11]. An excellent historical perspective of Schwarz methods may be found in [21]. Non-overlapping DDMs may also be defined. In non-overlapping methods the subdomains have empty intersection and exchange state and derivative information through their common interfaces. The first non-overlapping method was introduced in [26], and an a posteriori analysis of this method was presented in [8]. There are numerous other variants of non-overlapping methods e.g. Schur-complement and iterative substructuring [18, 30, 1] and Lagrange multiplier based substructuring methods [17, 16, 15, 27].

Adjoint-based a posteriori error analysis classically considers a differential equation,

\[ L(u) = g(x, t), \]

where \( L \) denotes the differential operator, and the error in a Quantity of Interest (QoI) expressed as a linear functional

\[ Q(u) = (u, \psi), \]

where \( \langle \cdot, \cdot \rangle \) denotes the \( L_2 \) inner product and \( \psi \) is chosen to yield the desired information. Given the numerical approximation \( U \) to the analytical solution, the residual \( R(U) = g - L(U) \) quantifies the effects of discretization on the evaluation of the differential equation, but it does not provide the error in the QoI. The relation between the residual and the error is derived from solving an adjoint problem.

\[ \text{The first mathematical formulation of DDMs dates much further back to Schwarz [31] who introduced the multiplicative overlapping DDM in 1870. Schwarz constructed solutions of partial differential equations (PDEs) in complicated geometries by decomposing the domain into simpler shapes on which the solution could be found analytically (e.g. by using separation of variables) and then defined an iteration which converged to the true solution under suitable conditions.} \]
For linear problems, the adjoint operator $L^* : Y^* \to X^*$ of a linear operator $L : X \to Y$ between Banach spaces $X, Y$ with dual spaces $X^*, Y^*$ is defined by the bilinear identity,

$$\langle Lx, y^* \rangle_Y = \langle x, L^*y^* \rangle_X, \quad x \in X, y^* \in Y^*,$$

(3)

where $\langle \cdot, \cdot \rangle_S$ denotes duality-pairing in the space $S \in \{X, Y\}$. The adjoint problem associated with (1) is

$$L^* \phi = \psi.$$  

(4)

This yields the error estimate,

$$\text{Error in the QoI} = (u - U, \psi) = (R(U), \phi).$$  

(5)

We use (5) by numerically solving the adjoint problem (4), computing the residual, and evaluating (5).

Adjoint-based a posteriori error analysis for systems of ordinary and partial differential equations has an extensive history [13, 12, 6, 19, 20, 4], and has been applied to a wide range of applications and numerical methods. Classical a posteriori error analysis for the numerical solution of differential equations assumes the use of fully implicit discretization methods in which the approximate solution is computed exactly and the adjoint of the forward operator [4] produces a useful adjoint solution. The adjoint of the discrete solution operator when implementing more complex, multistage solution methods is much more complicated to define. If the steps in the solution process are written as compositions of operators, then the appropriate adjoint can typically be written as a composition of adjoints associated with various steps of discretization. The resulting error estimate must then use the appropriate adjoint to weight specific residuals and include additional terms quantifying the difference between this adjoint and adjoints associated with various steps of discretization. The resulting error estimate then use the appropriate adjoint to weight specific residuals and include additional terms quantifying the difference between this adjoint and adjoints associated with various steps of discretization. The correct choice of adjoint and residuals also enables a decomposition of the total error in to distinct sources of error, such as discretization, iteration, transfer, projection and quadrature errors. These concepts are illustrated in an analysis of iterative solvers for non-autonomous evolution problems in [9] and in an analysis of an iterative multi-discretization method for reaction-diffusion systems in [7].

Adjoint-base a posteriori error estimates can provide useful information for designing efficient two stage solution strategies. During the first “pre-processing” stage, a solution is computed on a relatively coarse discretization together with an accurate a posteriori error estimate that quantifies the contributions of all sources of error. The information provided by the first stage is used to guide discretization choices for a second “production level” computation. This strategy is described in earlier work on blockwise adaptivity [6, 22] and in [10].

We introduce the multiplicative and additive Schwarz overlapping domain decomposition methods in [2]. Definitions of discretization and iteration errors appear in [3], as well as the adjoint problems and error representation formulas for both multiplicative and additive Schwarz. Numerical examples are provided for multiplicative Schwarz in [4] and for additive Schwarz in [5]. Details of the analysis appear in [6]. A discussion and future research directions appear in [7].

2 Overlapping Schwarz domain decomposition

Assume that we have $p$ overlapping subdomains $\Omega_1, \ldots, \Omega_p$ on a domain $\Omega$. That is, for any subdomain $\Omega_i$, there exists a subdomain $\Omega_j$, $i \neq j$ such that $\Omega_i \cap \Omega_j \neq \emptyset$ and $\Omega_i \cap \Omega_j = \Omega$. We denote by $L_2(\Omega)$ as the space of square integrable functions, $H^1(\Omega)$ as the space of functions having an integrable (weak) derivative and $H^1_0(\Omega)$ as the subspace of $H^1(\Omega)$ of functions satisfying homogeneous Dirichlet boundary conditions (in the sense of the trace operator). Let $\langle \cdot, \cdot \rangle$ and $\langle \cdot, \cdot \rangle_{ij}$ represent the $L_2(\Omega)$ and $L_2(\Omega_i \cap \Omega_j)$ inner products respectively.

The weak form of the PDE problem is to find $u \in H^1_0(\Omega)$ such that

$$a(u, v) = l(v) \quad \forall v \in H^1_0(\Omega).$$

(6)

Here $a(\cdot, \cdot)$ is the standard bilinear form over $\Omega$ arising from integration by parts of the PDE operator and $l(\cdot)$ is the linear functional arising from the right-hand-side of the PDE. For example, given the Poisson equation $-\nabla^2 u(x) = f(x)$ with homogeneous Dirichlet boundary conditions, we have $a(u, v) = \int_{\Omega} \nabla u \cdot \nabla v \, dx$ and $l(v) = (f, v)$.

We denote by $a_i(\cdot, \cdot)$ the restriction of $a(\cdot, \cdot)$ of over $\Omega_i$ and $a_{ij}(\cdot, \cdot)$ the restriction of $a(\cdot, \cdot)$ over $\Omega_i \cap \Omega_j$. Similarly, we let $l_i(\cdot)$ be the restriction of $l(\cdot)$ over $\Omega_i$.

We are interested in a QoI which is a linear functional of the solution and is represented as,

$$Q(u) = (\psi, u).$$

(7)

where $\psi \in L_2(\Omega)$. 
2.1 Multiplicative Schwarz overlapping domain decomposition

The multiplicative Schwarz method is given in Algorithm 1. Here $H^1_D(Ω_i) \equiv \{ v \in H^1(Ω_i) | v = u^{(k+i-1)/p} \text{ on } ∂Ω_i \}$. 

**Algorithm 1** Overlapping multiplicative Schwarz

Given $u^{(0)}$ defined on $Ω$.
for $k = 0, 1, 2, \ldots, K − 1$ do
  for $i = 1, 2, \ldots, p$ do
    Find $\tilde{u}^{(k+i)/p} \in H^1_D(Ω_i)$ such that 
    $$a_i(\tilde{u}^{(k+i)/p}, v) = l_i(v) \quad ∀v \in H^1_0(Ω_i) \quad (8)$$
  
  Let 
  $$u^{(k+i)/p} = \begin{cases} 
  \tilde{u}^{(k+i)/p} & \text{on } Ω_i \\
  u^{(k+i-1)/p} & \text{on } Ω \setminus Ω_i
  \end{cases} \quad (9)$$
end for
end for

2.2 Additive Schwarz overlapping domain decomposition

The basic additive Schwarz solution method is provided in Algorithm 2. Here $H^1_D(Ω_i) \equiv \{ v \in H^1_D(Ω_i) | v = u^{(k)} \text{ on } ∂Ω_i \}$, and $τ$ is the Richardson parameter, needed to ensure that the iteration converges [28].

**Algorithm 2** Overlapping additive Schwarz

Given $u^{(0)}$ defined on $Ω$.
for $k = 0, 1, 2, \ldots, K − 1$ do
  for $i = 1, 2, \ldots, p$ do
    Find $\tilde{u}_i^{(k+1)} \in H^1_D(Ω_i)$ such that 
    $$a_i(\tilde{u}_i^{(k+1)}, v) = l_i(v) \quad ∀v \in H^1_0(Ω_i). \quad (10)$$
  
  Let $Π\tilde{u}_i^{(k+1)} = \begin{cases} 
  \tilde{u}_i^{(k+1)} & \text{on } Ω_i \\
  u^{(k)} & \text{on } Ω \setminus Ω_i
  \end{cases}$.

  Let 
  $$u^{(k+1)} = (1 − τp)u^{(k)} + τ \left( ∑_{i=1}^{p} Π\tilde{u}_i^{(k+1)} \right). \quad (11)$$
end for
end for
2.3 Finite element discretizations

We let $T_h$ denote a quasi-regular triangulation of $\Omega$ such that no node of one element $T_i$ intersects an interior edge of another $T_j$ and $\Omega = \bigcup_m K_m$. Moreover, the triangulation is consistent in the sense that if $T_i \cap \Omega_j \neq \emptyset$ then $T_i \subset \Omega_j$.

We can represent the discretized version of the overlapping domain decomposition algorithm by substituting finite dimensional spaces $V_{i,h}^k$ in place $H^1_V(\Omega)$ and $V_{i,h,0}$ in place of $H^1_0(\Omega)$ in Algorithm 1. Here $V_{i,h}^k$ and $V_{i,h,0}$ refer to the standard nodal finite element spaces consisting space of continuous piecewise polynomial functions on $T_h$. Additionally denote $V_h \subset H^1_0(\Omega)$ as the standard nodal finite element spaces consisting space of continuous piecewise polynomial functions over $\Omega$.

We represent the global discrete solutions as $U^{(k+i/p)}_i$ (resp. $U^{(k)}_i$) belonging to the space $V_h$ and the local discrete solutions as $\bar{U}^{(k+i/p)}_i$ (resp. $\bar{U}^{(k)}_i$) belonging to the space $V_{i,h,0}$ for the multiplicative (resp. additive) Schwarz methods. For simplicity we assume that $U^{(0)} = u^{(0)}$, that is, the discrete initial guess is the same as the continuum initial guess. Note that for both algorithms, the global continuum (resp. discrete) solution after $K$ iterations is represented as $u^{(k)}$ (resp. $U^{(k)}$). This allows for simplicity of presentation for results which apply to both algorithms in Algorithm 2.

3 A posteriori analysis of Schwarz Algorithms

The aim of this section is to derive the representation formula for the error in the QoI (7) that is computed from the discrete solution of the multiplicative or additive domain decomposition method after $K$ iterations. That is, we use adjoint-based analysis to find an error representation for $Q(u) - Q(U^{(K)}) = (\psi, u - U^{(K)})$.

3.1 The total error and its components

3.1.1 The total error

We define the global adjoint
\[
a(v, \phi) = (\psi, v) \quad \forall v \in H_0^1(\Omega),
\]
and obtain a representation for total error as below.

**Theorem 1** (Total error representation.). The error in the QoI for the discretized multiplicative or additive Schwarz algorithm after $K$ iterations is given by,
\[
(u - U^{(K)}), \psi) = R(U^{(K)}, \phi)
\]
where $R(U^{(K)}, \phi) = l(\phi) - a(U^{(K)}, \phi)$ is the weak residual.

The proof of Theorem 1 is standard, see e.g., [12]. Theorem 1 gives the error in the QoI, however, it does not capture the structure of the differential operator corresponding to the Schwarz domain decomposition. Performing Schwarz domain decomposition with a finite number of iterations, as in Algorithms 1 and 2, defines a differential operator which is distinct from the differential operator associated with the original PDE (6). The numerical solution $U^{(K)}$ is a solution to the discretization of this modified operator. Hence, a more sophisticated analysis that takes into account the modified operator is required. We carry out this analysis by decomposing the error into two components: iterative and discretization errors. Moreover, we note that for implementation purposes, the global adjoint $\phi$ may be approximated by a Schwarz domain decomposition method.

3.1.2 Discretization and iteration errors

We decompose the total error as,
\[
u - U^{(K)} = \underbrace{u - u^{(K)}}_{\text{Iteration Error}} + \underbrace{u^{(K)} - U^{(K)}}_{\text{Discretization Error}} = e_I^{(K)} + e_D^{(K)},
\]
where $e_I^{(k)} = u - u^{(k)}$ and $e_D^{(k)} = u^{(k)} - U^{(k)}$. Since $U^{(0)} = u^{(0)}$, we have $e_D^{(0)} = 0$. The iteration error captures the error due to the discrepancy between the PDE differential operator and the modified differential operator in the Schwarz algorithms arising from using a finite number of $K$ iterations. The discretization error represents the error between the analytical solution to the modified differential operator and the numerical approximation to this modified operator.

The iteration error is given by the difference of the total and discretization errors.
Theorem 2 (Iteration error representation).

\[(u - u^{(K)}), \psi\] = \(R(U^{(K)}, \phi) - (\psi, u^{(K)} - U^{(K)})\)  \hspace{1cm} (15)

Proof. This follows by combining [13] and [14].

The analysis of the discretization error involves partitioning of the QoI data over subdomains by a partition of unity. Similar ideas to use a partition of unity in the context of adjoint based analysis is present in [14]. Let \(\chi_i\) be a partition of unity such that

\[\psi_i = \chi_i \psi,\] (16)

and \(\psi_i = 0\) on \(\Omega \setminus \Omega_i\). The partition of unity localizes the QoI data, and hence the error, to a particular subdomain. Such a partition of unity may be constructed in different ways. We illustrate one such example of a partition of unity that is also used in the numerical examples. Let \(d_i(x)\) denote the distance function:

\[d_i(x) = \begin{cases} \text{dist}(x, B^{(i)}) & \text{if } x \in \overline{\Omega_i} \\ 0 & \text{if } x \notin \overline{\Omega_i} \end{cases},\] (17)

where \(B^{(i)} = (\partial \Omega_i \cap \Omega)\). Then set,

\[\chi_i(x) = \frac{d_i(x)}{\sum_{j=1}^{p} d_j(x)}.\] (18)

With this partition of the QoI data, we have the following partition of the QoI.

Lemma 1 (Partitioning the QoI data over subdomains). We have,

\[(e^{(k)}_D, \psi) = \sum_{i=1}^{p} (e^{(k)}_D, \psi_i)_{ii}.\] (19)

Proof. This follows directly from the definition of the partition of unity in [16].

\[(e^{(k)}_D, \psi) = (e^{(k)}_D, \sum_{i=1}^{p} \chi_i \psi) = \sum_{i=1}^{p} (e^{(k)}_D, \psi_i)_{ii}.\]

3.1.3 Weak Residuals

Appropriately defined residuals play an important role in adjoint based error analysis. We define the subdomain weak residuals as

\[R_i(s, v) = l_i(v) - a_i(s, v),\] (20)

for \(i = 1, 2, \ldots, p\).

3.2 A posteriori error analysis of discretization error for multiplicative Schwarz

In this section we derive representation of the discretization error in the QoI obtained from the multiplicative Schwarz method in Algorithm [4]. That is, we use adjoint based analysis to compute \((\psi, u^{(K)} - U^{(K)})\).

3.2.1 Adjoint problems for discretization error

Define adjoints \(\phi^{[k+i/p]}\) belonging to \(H^1(\Omega_i)\) as follows:

\[a_i(v, \phi^{[Q+i/p]}) = t^Q_i(v) - \sum_{j=i+1}^{p} a_{ij}(v, \phi^{[Q+j/p]}) \quad \forall v \in H^1(\Omega_i),\] (21)
where
\[
\tau_i^Q(v) = \begin{cases} 
\sum_{j=1}^{p} (v, \psi_j)_{ij}, & Q = K - 1, \\
- \sum_{j=1}^{p} a_{ij}(v, \phi^{[Q+1+j/p]}), & 0 \leq Q < K - 1.
\end{cases}
\]  \hspace{1cm} (22)

The right hand side of (21) captures not only the localized QoI data (in the form of \((v, \psi_j)_{ij}\)), but also the transfer error between subdomains as the iteration proceeds (in the form of \(- \sum_{j=1}^{p} a_{ij}(v, \phi^{[Q+1+j/p]}))\). The adjoint problems (21) have the same nature of sequential subdomains solve as the multiplicative Schwarz Algorithm [1] but note that these are defined backwards from \(K\), \(K - 1 + (p - 1)/p\), \(K - 1 + \frac{m}{p}, \ldots, 1\).

### 3.2.2 Discretization error

**Theorem 3** (Discretization error for multiplicative Schwarz). The discretization error in the QoI for the multiplicative Schwarz Algorithm [2] is,

\[
(\psi, u^{[K]} - U^{[K]}) = \sum_{k=0}^{K-1} \sum_{i=1}^{p} R_i(U^{[k+i/p]}, \phi^{[k+i/p]} - \pi \phi^{[k+i/p]}).
\]  \hspace{1cm} (23)

where \(\pi : H^1_0(\Omega_i) \rightarrow V_{i,h,0}\) represents a projection operator.

The proof of Theorem 3 depends on a number of technical lemmas. The details of the lemmas and their proofs are given in [6.1]. The presence of the term \((\phi^{[k+i/p]} - \pi \phi^{[k+i/p]})\) arises from the use of Galerkin orthogonality. Galerkin orthogonality represents the fact that the residual of the discrete solution is zero on the finite dimensional space \(V_{i,h,0}\), that is, the \(U^{[k+i/p]}\) is the discrete approximation to the analytical solution \(u^{[k+i/p]}\) and not to the solution \(u\). This is the reason that the basic error representation [13] lacks the use of Galerkin orthogonality.

### 3.3 A posteriori analysis of discretization error for additive Schwarz

In this section we derive representation of the discretization error in the QoI obtained from the additive Schwarz method in Algorithm [2].

#### 3.3.1 Adjoint problems for discretization error

Define adjoints \(\phi_i^{[k]}\) belonging to \(H^1_0(\Omega_i)\) as follows:

\[
a_i(v, \phi_i^{[k]}) = \sum_{j=1}^{p} \left[ (\psi_j, v)_{ij} - a_{ij} \left( v, \sum_{l=k+1}^{K} \phi_j^{[l]} \right) \right], \quad \forall v \in H^1_0(\Omega_i).
\]  \hspace{1cm} (24)

Given a fixed \(k\), the adjoint problems \(\phi_i^{[k]}\) in (24) are independent for each \(i\). That is, for a fixed \(k\), \(\phi_i^{[k]}\) may be computed in parallel analogous to the solution strategy in the additive Schwarz Algorithm [2]. However, these are defined backwards from \(K\), \(K - 1\), \(K - 2\), \ldots, 1. We also note that for implementation purposes \(\sum_{l=k+1}^{K} \phi_j^{[l]}\) involves a sum of the two vectors, \(\sum_{l=k+2}^{K} \phi_j^{[l]}\) (which has already been computed earlier) and \(\phi_j^{[k+1]}\).

#### 3.3.2 Discretization error

**Theorem 4** (Discretization error for additive Schwarz). The discretization error in the QoI for the additive Schwarz Algorithm [2] is,

\[
(\psi, e^{[K]}_D) = (\psi, u^{[K]} - U^{[K]}) = \sum_{k=1}^{K} \sum_{i=1}^{p} R_i(U_i^{[k]}, \phi_i^{[k]} - \pi \phi_i^{[k]}).
\]  \hspace{1cm} (25)

The proof of Theorem 4 depends on a number of technical lemmas. The details of the lemmas and their proofs appear in [6.2].
3.4 Solution algorithms

The full algorithm for a posteriori error estimation for overlapping multiplicative/additive Schwarz domain decomposition is provided in Algorithm 3.

Algorithm 3
Adjoint-based a posteriori error estimation procedure for overlapping multiplicative DD

\[
\text{for } k = 0,1,2,\ldots,K-1 \text{ do}
\]

\[
\text{for } i = 1,2,\ldots,p \text{ do}
\]

Solve primal problem on subdomain \(i\)

Combine to construct a global solution

(see (8)/(10))

(see (9)/(11))

end for

end for

\[
\text{for } k = K-1,K-2,\ldots,0 \text{ do}
\]

\[
\text{for } i = p,p-1,\ldots,1 \text{ do}
\]

Solve adjoint on subdomain \(i\)

Compute adjoint weighted residuals and accumulate error contributions

(see (21)/(24))

(see (23)/(25))

end for

end for

Solve global adjoint

Calculate total error

Calculate iteration error

(see (12))

(see (13))

(see (15))

4 Numerical examples for multiplicative Schwarz

4.1 Error estimates and effectivity ratios

The adjoint solutions are also approximated in a discrete setting. Let \(\Phi^{(k+i/p)}\) be the discrete approximation to \(\phi^{(k+i/p)}\), and \(\Phi\) the discrete approximation to \(\phi\). Then, we obtain error estimates from error representations (23) and (13). These error estimates are,

\[
\eta^K_D = \sum_{k=0}^{K-1} \sum_{i=1}^{p} R_i(U^{(k+i/p),\Phi^{[k+i/p]}}) \quad (26)
\]

and

\[
\eta^K = R(U^{(K)},\Phi) \quad (27)
\]

The performance of an error estimate is measured by the effectivity ratio. Effectivity ratio for total error is,

\[
\gamma = \frac{\eta^K}{(u - U^{(K)},\psi)} \quad (28)
\]

Effectivity ratio for discretization error is,

\[
\gamma_D = \frac{\eta^K_D}{(u^{(K)} - U^{(K)},\psi)} \quad (29)
\]

An effectivity ratio close to one indicates that the error estimate is accurate. We also recall that \(\epsilon_I\) denotes the iteration error.

4.2 Estimates for Poisson’s equation

Consider the Poisson’s equation

\[
-\nabla^2 u = f \quad \text{in } \Omega, \\
u = 0 \quad \text{on } \partial\Omega, \quad (30)
\]

in a square domain \(\Omega = [0.0, 1.0] \times [0.0, 1.0]\), where \(f(x,y) = 8\pi^2 \sin(2\pi x) \sin(2\pi y)\). In the computations below, unless otherwise specified, the mesh is uniform and contains \(2 \times N_x \times N_y\) triangular elements. The overlap between subdomains is indicated by \(\beta\).
4.2.1 \( 2 \times 1 \) subdomains

Two overlapping subdomains \( \Omega_1 = [0.0, 0.6] \times [0.0, 1.0] \) and \( \Omega_2 = [0.4, 1.0] \times [0.0, 1.0] \) are illustrated in Figure 1a corresponding to an overlap parameter \( \beta = 0.1 \). The solid black lines in this figure and in subsequent figures, indicate the mid-distance between overlapping subdomains. The QoI in (7) is specified by

\[
\psi = 1_{[0.6, 0.8] \times [0.6, 0.8]}
\]

where \( 1_\omega \) is the characteristic function on a domain \( \omega \).

Estimates of the discretization, iteration and total errors, and the corresponding effectivity ratios varying the overlap \( \beta \), number of Schwarz iterations \( K \) and number of elements are shown in Tables 1. In all cases the effectivity ratios are close to 1.0. The table highlights the sensitivity of our estimates to the distinct components of error. The “base” computation with \( N_x = N_y = 20, \beta = 0.1 \) and \( K = 2 \) is repeated for ease of comparison. Increasing the overlap decreases the iteration error \( e_I^{(K)} \) but does not have a significant effect on the discretization error \( e_D \).

The iteration error decreases with increasing number of Schwarz iterations, but the discretization error is largely unaffected. The discretization error decreases when the mesh is refined but the iteration error remains essentially constant.

| \( N_x \) | \( N_y \) | \( \beta \) | \( K \) | Est, Err | \( \gamma \) | \( e_I^{(K)} \) | \( \gamma_D \) | \( e_D \) |
|---|---|---|---|---|---|---|---|---|
| 20 | 20 | 0.1 | 2 | 1.02e-03 | 9.98e-01 | 6.56e-04 | 9.98e-01 | 3.60e-04 |
| 20 | 20 | 0.2 | 2 | 7.03e-04 | 9.96e-01 | 6.28e-04 | 9.97e-01 | 7.50e-05 |
| 20 | 20 | 0.1 | 4 | 6.55e-04 | 9.96e-01 | 6.26e-04 | 9.97e-01 | 2.89e-05 |
| 20 | 20 | 0.1 | 2 | 1.02e-03 | 9.98e-01 | 6.56e-04 | 9.98e-01 | 3.60e-04 |
| 40 | 40 | 0.1 | 2 | 5.25e-04 | 1.00e+00 | 1.66e-04 | 9.99e-01 | 3.60e-04 |

Table 1: Multiplicative Schwarz for Poisson’s equation: \( 2 \times 1 \) domains.

4.2.2 \( 4 \times 1 \) subdomains

The computational domains for \( \beta = 0.1 \) are shown in Figure 1b. We choose the same QoI as before as given by equation (31). It is well known that as the number of domains increase, the convergence of Schwarz methods decreases and this is evident by comparing Tables 2 and 1. While the discretization errors are of comparable magnitude between the four subdomain and two subdomains case, the iteration error \( e_I^{(K)} \) is an order of magnitude larger given four subdomains as compared to two. The contributions of the separate components of the total error vary with the overlap, number of iterations and number of elements in a qualitatively similar way to that discussed above in § 4.2.1.
## 4.2.3 4 × 4 subdomains

The computational domains for \( \beta = 0.1 \) and sixteen equally-sized subdomains configured as a \( 4 \times 4 \) grid is shown in Figure 2a. The error estimates for QoI given by equation (31) are again quite accurate as evidenced by effectivity ratios close to 1.0. The results, shown in Table 3 are again qualitatively similar to those in Tables 1 and 2. The iteration error is even larger for this scenario that in the \( 4 \times 1 \) case, while the discretization errors are essentially the same as both the \( 2 \times 1 \) and \( 4 \times 1 \) cases, as is to be expected when the finite element mesh is the same.

| \( N_x \) | \( N_y \) | \( \beta \) | \( K \) | Est. Err. | \( \gamma \) | \( e_D^{(K)} \) | \( \gamma_D \) | \( e_I^{(K)} \) |
|-------|-------|-----|-----|-------|-----|-------|-----|-------|
| 20    | 20    | 0.1 | 2   | 4.57e-03 | 9.99e-01 | 6.92e-04 | 9.97e-01 | 3.88e-03 |
| 20    | 20    | 0.2 | 2   | 1.34e-03 | 9.98e-01 | 6.48e-04 | 9.98e-01 | 6.87e-04 |
| 20    | 20    | 0.1 | 2   | 4.57e-03 | 9.99e-01 | 6.92e-04 | 9.97e-01 | 3.88e-03 |
| 20    | 20    | 0.1 | 4   | 1.04e-03 | 9.98e-01 | 6.48e-04 | 9.98e-01 | 3.94e-04 |
| 20    | 20    | 0.1 | 2   | 4.57e-03 | 9.99e-01 | 6.92e-04 | 9.97e-01 | 3.88e-03 |
| 40    | 40    | 0.1 | 2   | 4.05e-03 | 1.00e+00 | 1.75e-04 | 9.99e-01 | 3.88e-03 |

Table 2: Multiplicative Schwarz for Poisson’s equation: \( 4 \times 1 \) domains.

### 4.3 Cancellation of error

To demonstrate the potential for cancellation between discretization and iteration errors, the quantity of interest is chosen to be

\[
\psi = \chi_{[0.4, 0.8] \times [0.4, 0.8]}
\] (32)

for two subdomains and an overlap \( \beta = 0.05 \). Computational results for an increasing number of Schwarz iterations are shown in Table 3. The magnitude of the total error initially decreases as the iteration proceeds, reaching a minimum after six iterations, but then starts to increase. This behavior would be surprising at first glance but is well-explained by observing that the discretization and iteration errors have opposite signs. The discretization error is essentially fixed as the iteration proceeds and has a value of \(-1.6 \times 10^{-4}\). The initial iteration error is of order \(4.0 \times 10^{-3}\) and the iteration error dominates the total error. As expected, the iteration error decreases monotonically as \( K \) increases, but is always positive. After six iterations the discretization and iteration errors have approximately equal magnitudes but opposite signs opposite signs, and cancel to produce a total error of \(3.0 \times 10^{-5}\). For greater than six iterations, the iteration error continues to decrease but now the discretization error dominates the total error. The total error increases to \(-1.5 \times 10^{-4}\) after 10 iterations and will gradually approach the (fixed) discretization error as the number of iterations increases further.

| \( N_x \) | \( N_y \) | \( \beta \) | \( K \) | Est. Err. | \( \gamma \) | \( e_D^{(K)} \) | \( \gamma_D \) | \( e_I^{(K)} \) |
|-------|-------|-----|-----|-------|-----|-------|-----|-------|
| 20    | 20    | 0.1 | 2   | 9.22e-03 | 1.00e+00 | 1.02e-03 | 1.00e+00 | 8.20e-03 |
| 20    | 20    | 0.2 | 2   | 2.80e-03 | 9.99e-01 | 7.31e-04 | 9.98e-01 | 2.07e-03 |
| 20    | 20    | 0.1 | 2   | 9.22e-03 | 1.00e+00 | 1.02e-03 | 1.00e+00 | 8.20e-03 |
| 20    | 20    | 0.1 | 4   | 2.72e-03 | 9.99e-01 | 8.27e-04 | 9.99e-01 | 1.90e-03 |
| 20    | 20    | 0.1 | 2   | 9.22e-03 | 1.00e+00 | 1.02e-03 | 1.00e+00 | 8.20e-03 |
| 40    | 40    | 0.1 | 2   | 8.45e-03 | 1.00e+00 | 2.55e-04 | 1.00e+00 | 8.20e-03 |

Table 3: Multiplicative Schwarz for Poisson’s equation: \( 4 \times 4 \) domains.
Consider the convection-diffusion equation

\[-\nabla^2 u + b \cdot \nabla u = f \quad \text{in } \Omega,\]
\[u = 0 \quad \text{on } \partial\Omega,\]  
(33)

where \(\Omega = [0.0, 1.0] \times [0.0, 1.0]\), \(f(x, y) = 1\), and \(b = [-60, 0]\). The effect of this convective vector field is to carry information from right to left. For this example, we choose the quantity of interest

\[\psi = 1_{[0.05, 0.2] \times [0.05, 0.2]},\]  
(34)

which is concentrated near the bottom left hand corner. The adjoint problems were solved using continuous piecewise cubic polynomials to ensure accurate solutions in the presence of the strong convective vector field. We experiment with two configurations with the subdomains aligned with different coordinate axes, and either parallel with or perpendicular to the direction of convection.

### 4.4.1 4 \times 1 configuration

This subdomain configuration is the same as in Figure 1b. The total, discretization and iteration errors are provided in Table 5. Note the significant iteration error in this configuration for \(K = 2\), which dominates the total error. The large iteration error for \(K = 2\) is to be expected given the direction of information travel from right to left. The iteration error decreases dramatically for \(K = 4\) and \(K = 6\), once information has traveled across the subdomains, and discretization error becomes the dominant error.

### 4.4.2 1 \times 4 configuration

This subdomain configuration is shown in Figure 1c and now the subdomains are aligned with the direction of the convective vector field. The iteration error after two iterations and the total error are more than an order of magnitude less than in the 4 \times 1 case. In this scenario, one subdomain contains most of the “domain of influence” for the QoI and hence results in low iteration error, even for \(K = 2\). There is again fortuitous cancellation between the discretization and iteration errors for \(K = 2\) so that the total error increases for \(K = 4\) and \(K = 6\) with the total error dominated by the discretization error.
4.5 Two stage solution strategy for Poisson’s equation

Adjoint-base *a posteriori* error estimates can provide useful information in designing efficient two stage strategies. First, a preliminary, inexpensive computation is performed with potentially large error. This “stage 1” solution is analyzed and the different error components determined. A production, more expensive “stage 2” calculation is then performed with different numerical parameters that have been chosen to address the main causes of error. We provide two examples of this strategy below where the dominant error in the stage 1 calculation is differs. The “stage 1” calculation for both experiments were run on a $2 \times 2$ subdomain configuration as shown in Figure 2b.

4.5.1 Discretization error dominant in stage 1

Consider again the QoI given by (31). The results on the initial $2 \times 2$ subdomain configuration with $N_x = N_y = 10, \beta = 0.2$ and $K = 6$ are provided in Table 6. The main source of the error is the discretization error $e^{D}_1$. In order to reduce the discretization error, we need to reduce the discretization error contribution arising from each subdomain. We define the contribution to the discretization error from subdomain $i$ as

$$S^K_i = \sum_{k=0}^{K-1} R_i(U^{\{k+i/p\}}, \phi^{[k+i/p]} - \pi \phi^{[k+i/p]}), \quad i = 1, \ldots, p,$$

so that the discretization error, (23) may be written as,

$$(\psi, u^K - U^K) = \sum_{i=1}^{P} S^K_i.$$  

The values of $S^K_i$ are also shown in Table 6. Subdomain 4 contributes the most towards the discretization error, and we refine all the elements in this domain. The results for the error and the values of $S^K_i$ after the refinement are shown in Tables 6. The discretization error is significantly lower and hence the total error is also significantly lower. Furthermore, the values of $R^K_i$ also indicate that now each subdomain contributes roughly the same magnitude towards the discretization error. We also note that uniformly refining the (initial) mesh results in a refined mesh with 441 vertices and an error of 6.24e−04. This uniformly mesh has almost twice the number of degree of freedoms than the refined mesh of Table 6 but still has twice the error, indicating how the error contributions can help in deciding numerical parameters for efficient simulation.
4.5.2 Iteration error dominant in stage 1

For the same choice of QoI, we perform a stage 1 computation with \(2 \times 2\) subdomains and \(N_x = N_y = 40\), \(\beta = 0.05\) and \(K = 2\). The contributions to the total error are shown in Table 7. The dominant source of the error is the iteration error \(e_i^{(K)}\). There are two ways to reduce it, either by performing a great number of iterations or increasing \(\beta\). We choose the latter option and the results are shown in Table 7, where now the iteration error and discretization are balanced and the overall error has decreased.

Table 6: Two stage solution strategy using multiplicative Schwarz to solve Poisson’s equation: \(\beta = 0.2\), \(K = 6\). Stage 1: number of vertices = 121. Stage 2: number of vertices = 253.

### Numerical examples for additive Schwarz

We largely repeat the numerical examples in §4 for additive Schwarz. Effectivity ratios for the discretization error and the total error are defined analogously to the case of the multiplicative Schwarz case by replacing \(\Phi_{k+i/p}\) in the above expressions by \(\Phi_k\) in the expressions in §4.1, where \(\Phi_k\) is the numerical approximation to \(\phi_k\). The error estimates are again quite accurate with effectivity ratios close to 1.

### Estimates for Poisson’s equation

#### 2 \(\times\) 1 subdomains

We solve the same problem described in §4.2.1 by equations (30) and (31) using additive Schwarz. The results are shown in Table 8. In comparison to the results in §4.2.1, we observe that the additive Schwarz method has much higher iteration error than multiplicative Schwarz method. The discretization error is of course approximately the same.

Table 7: Two stage solution strategy using multiplicative Schwarz to solve Poisson’s equation. Stage 1: \(\beta = 0.05\), stage 2: \(\beta = 0.2\).

Table 8: Additive Schwarz for Poisson’s equation: \(2 \times 1\) domains.

#### 4 \(\times\) 1 subdomains

The results solving the same problem using twice the number of subdomains are shown in Table 9. The iteration error is considerably larger than for multiplicative Schwarz and the convergence rate with increasing numbers of iterations appears to be much slower. The discretization error is again approximately the same.
Table 9: Additive Schwarz for Poisson’s equation: 4 × 1 domains.

5.1.3 4 × 4 subdomains

Repeating the problem in §4.2.3 and using additive Schwarz produces the results provided in Table 10.

Table 10: Additive Schwarz for Poisson’s equation: 4 × 4 domains.

Once again the iteration error is significantly greater than in the multiplicative case and appears to improve more slowly with increasing overlap or number of iterations.

5.2 A convection-diffusion problem

The problem formulation is defined in §4.4 by equations (33) and (34). We provide results for two different configurations of the subdomains in Table 11 below.

Table 11: Additive Schwarz for convection-diffusion: $N_x = N_y = 20$, $\beta = 0.1$.

The differences between these two configurations are not as dramatic as in the case of multiplicative Schwarz. Furthermore, both 4 × 1 and 1 × 4 configurations had essentially converged after 6 iterations of multiplicative Schwarz. This is far from true for additive Schwarz.

5.3 Two stage solution strategy for Poisson’s equation

5.3.1 Discretization error dominant in stage 1

Numerical results for the same convection diffusion problem as studied in §4.5.1 are shown in Table 12 below and similar conclusions may be drawn.
### Table 12: Two stage solution strategy using additive Schwarz to solve Poisson’s equation: $\beta = 0.2$, $K = 6$. Stage 1: number of vertices = 121. Stage 2: number of vertices = 253.

| Stage | Est. Err. | $\gamma$ | $\epsilon_D^{(K)}$ | $\gamma_D$ | $\epsilon_I^{(K)}$ |
|-------|-----------|-----------|---------------------|-----------|---------------------|
| 1     | 3.24e-03  | 9.88e-01  | 2.48e-03            | 9.90e-01  | 7.61e-04            |
| 2     | 1.24e-03  | 1.00e+00  | 4.79e-04            | 1.04e+00  | 7.60e-04            |

5.3.2 Iteration error dominant in stage 1

We repeat the problem described in §4.5.2 for which the iteration error is the dominant error. The results are shown in Table 13 below and again we observe the efficacy of the two-stage strategy.

| $N_x$ | $N_y$ | $\beta$ | $K$ | Est. Err. | $\gamma$ | $\epsilon_D^{(K)}$ | $\gamma_D$ | $\epsilon_I^{(K)}$ |
|-------|-------|---------|-----|-----------|-----------|---------------------|-----------|---------------------|
| 40    | 40    | 0.05    | 2   | 1.05e-02  | 1.00e+00  | 1.19e-04            | 1.00e+00  | 1.04e-02            |
| 40    | 40    | 0.2     | 2   | 8.27e-03  | 1.00e+00  | 1.15e-04            | 1.00e+00  | 8.15e-03            |

Table 13: Two stage solution strategy using additive Schwarz to solve Poisson’s equation. Stage 1: $\beta = 0.05$, stage 2: $\beta = 0.2$.

6 Details of analysis: algorithm reformulation, technical lemmas and proofs

6.1 Details of analysis of multiplicative Schwarz algorithm

6.1.1 Reformulation of the algorithm

Algorithm 1 is not amenable to adjoint based analysis since the affine solution space $H^1_{D_k}(\Omega_i)$ changes at every iteration. We reformulate the algorithm by using a standard lifting technique to account for this in Algorithm 4.

We set

$$\bar{u}^{(k+i/p)} = u^{(k+i/p)} + u^{(k+(i-1)/p)} \quad \text{on} \quad \Omega_i$$

(37)

where now $u^{(k+i/p)} \in H_0^1(\Omega_i)$.

**Algorithm 4** Reformulated overlapping multiplicative Schwarz

Given $u^{(0)}$ defined on $\Omega$.

For $k = 0, 1, 2, \ldots, K-1$ do

For $i = 1, 2, \ldots, p$ do

Find $u^{(k+i/p)} \in H_0^1(\Omega_1)$ such that

$$a_i(u^{(k+i/p)}, v) = l_i(v) - a_i(u^{(k+(i-1)/p)}, v) \quad \forall v \in H_0^1(\Omega_i)$$

(38)

Let

$$u^{(k+i/p)} = \begin{cases} 
  w^{(k+(i-1)/p)} + w^{(k+i/p)} & \text{on} \quad \Omega_i \\
  w^{(k+(i-1)/p)} & \text{on} \quad \Omega \setminus \Omega_i 
\end{cases}$$

(39)

end for

end for
There is an equivalent reformulation of the discrete Algorithm 1 as Algorithm 2 involving finite dimensional FEM spaces. We denote the unknown solutions in this case as $W^{(k+i)/p}$ belonging to the spaces $V_{i,h,0} \subset H^1_0(\Omega_i)$. Note that the solutions $W^{(k+i)/p}$ are devices for the analysis of the algorithm and are not computed in practice.

To distinguish between different solutions (true, analytical, discrete) we use the notation in Table 14.

### Table 14: Multiplicative Schwarz: notation for different solutions and their spaces.

| Notation | Formula | Space | Meaning |
|----------|---------|-------|---------|
| $u$ | $u^{(k)}$ | $H^1_0(\Omega)$ | True solution |
| $U^{(k)}$ | | $H^1_0(\Omega_i)$ | Global analytic solution at iteration $k$ |
| $\tilde{u}^{(k+i)/p}$ | $\tilde{U}^{(k+i)/p}$ | $H^{1,k}_D(\Omega_i)$ | Analytic solutions on $\Omega_i$ at iteration $k$ |
| $V_{i,h,0}$ | | $V^k_{i,h}$ | Discrete solutions on $\Omega_i$ at iteration $k$ |
| $w^{(k+i)/p}$ | $W^{(k+i)/p}$ | $H^1_0(\Omega_i)$ | Analytic solutions on $\Omega_i$ with homogeneous bcs at iteration $k$ |
| $\{u\}_K$ | | $H^1_0(\Omega_i)$ | Discrete solutions on $\Omega_i$ with homogeneous bcs at iteration $k$ |
| $e^{(k)}$ | $u - U^{(k)}$ | $H^1_0(\Omega)$ | Total error |
| $e^{(k)}$ | $u - \tilde{u}^{(k+i)/p}$ | $H^1_0(\Omega)$ | Global iteration error at iteration $k$ |
| $e^{(k)}$ | $\tilde{u}^{(k)} - U^{(k)}$ | $H^1_0(\Omega)$ | Global discretization error at iteration $k$ |
| $e^{(k+i)/p}_w$ | $w^{(k+i)/p} - W^{(k+i)/p}$ | $H^1_0(\Omega_i)$ | Discretization error on $\Omega_i$ with homogeneous bcs at iteration $k$ |

### 6.1.2 Technical lemmas

Let $e^{(k)}_w = w^{(k)} - W^{(k)}$. By (37) we have

$$e^{(k+i)/p}_w = e^{(k+i)/p}_D - e^{(k+(i-1)/p)}_D \quad \text{on } \Omega_i$$

(40)

Note that $e^{(k+i)/p}_w = 0$ on $\partial \Omega_i$. We set $e^{(k+i)/p}_w = 0$ on $\Omega \setminus \Omega_i$.

**Lemma 2** (Error in QoI in terms of discretization errors with homogeneous boundary conditions). The discretization error in the QoI is

$$(e^{(K)}_D, \psi) = \sum_{k=0}^{K-1} \sum_{i=1}^{p} \sum_{j=1}^{p} (e^{(k+i)/p}_w, \psi_j)_{ij}.$$  

(41)

**Proof.** From equation (40) and the fact that $\psi_j = 0$ on $\Omega \setminus \Omega_j$ for fixed $j$ we have,

$$(e^{(K)}_D, \psi_j) = (e^{(K-1+i)/p}_D, \psi_j)$$

$$= (e^{(K-1+i)/p}_w, \psi_j)_{pj} + (e^{(K-1+i-(p-1)/p)}_D, \psi_j)$$

$$= (e^{(K-1+i)/p}_w, \psi_j)_{pj} + (e^{(K-1+(p-1)/p)}_w, \psi_j)_{(p-1)j} + (e^{(K-1+(p-2)/p)}_w, \psi_j).$$

(42)

Continuing,

$$(e^{(K)}_D, \psi_j) = (e^{(K-1)}_D, \psi_j) + \sum_{i=1}^{p} (e^{(K-1+i)/p}_w, \psi_j)_{ij}. \quad (43)$$

This is a recursive relation for $e^{(K)}_D$. Expanding $(e^{(K-1)}_D, \psi_j)$ as above leads to

$$(e^{(K)}_D, \psi_j) = \sum_{k=0}^{K-1} \sum_{i=1}^{p} (e^{(k+i)/p}_w, \psi_j)_{ij}. \quad (44)$$

Summing over $j = 1, \ldots, p$,

$$\sum_{j=1}^{p} (e^{(K)}_D, \psi_j) = \sum_{k=0}^{K-1} \sum_{i=1}^{p} \sum_{j=1}^{p} (e^{(k+i)/p}_w, \psi_j)_{ij}. \quad (45)$$
Lemma 3 (Bilinear form with discretization errors with homogeneous boundary conditions). For any \( v \in H^1_D(\Omega_i) \) we have
\[
a_i(e_D^{(i/p)}, v) = a_i(e_D^{(i/p)}, v) - \sum_{r=1}^{i-1} a_{ir}(e_W^{(r/p)}, v),
\]
and for \( k \geq 1 \),
\[
a_i(e_W^{(k+i/p)}, v) = a_i(e_D^{(k+i/p)}, v) - a_i(e_D^{(k-1+i/p)}, v) - \sum_{r=1}^{i-1} a_{ir}(e_W^{(k+r/p)}, v) - \sum_{r=i+1}^{p} a_{ir}(e_W^{(k-1+r/p)}, v).
\]

Proof. By (40) we have for \( m < i \),
\[
a_i(e_D^{(m/p)}, v) = a_i(e_D^{(m-1/p)}, v) + a_{i,m}(e_W^{(m/p)}, v),
\]
where we used \( e_W^{(r/p)} = 0 \) on \( \Omega \setminus \Omega_r \). Continuing in this manner leads to,
\[
a_i(e_D^{(m/p)}, v) = a_i(e_D^{(0)}, v) + \sum_{r=1}^{m} a_{ir}(e_W^{(r/p)}, v) = \sum_{r=1}^{m} a_{ir}(e_W^{(r/p)}, v),
\]
thus showing (46). A similar argument shows (47) for \( k \geq 1 \).

Lemma 4 (Sums of bilinear form with discretization errors with homogeneous boundary conditions). For \( 0 \leq Q \leq K - 1 \) we have
\[
\sum_{k=0}^{Q} a_i(e_W^{(k+i/p)}, v) = a_i(e_D^{(Q+i/p)}, v) - \sum_{k=0}^{Q} \sum_{r=1}^{i-1} a_{ir}(e_W^{(k+r/p)}, v) - \sum_{k=0}^{Q-1} \sum_{r=i+1}^{p} a_{ir}(e_W^{(k-1+r/p)}, v).
\]

Proof. By Lemma 3
\[
\sum_{k=0}^{Q} a_i(e_W^{(k+i/p)}, v) = \sum_{k=1}^{Q} a_i(e_W^{(k+i/p)}, v) + a_i(e_W^{(i/p)}, v)
\]
\[
= \sum_{k=1}^{Q} \left[ a_i(e_D^{(k+i/p)}, v) - a_i(e_D^{(k-1+i/p)}, v) - \sum_{r=1}^{i-1} a_{ir}(e_W^{(k+r/p)}, v) - \sum_{r=i+1}^{p} a_{ir}(e_W^{(k-1+r/p)}, v) \right]
\]
\[
+ a_i(e_D^{(i/p)}, v) - \sum_{r=1}^{i-1} a_{ir}(e_W^{(r/p)}, v)
\]
\[
= \sum_{k=1}^{Q} \left[ a_i(e_D^{(k+i/p)}, v) - a_i(e_D^{(k-1+i/p)}, v) \right] + a_i(e_D^{(i/p)}, v)
\]
\[
- \sum_{k=1}^{Q} \sum_{r=1}^{i-1} a_{ir}(e_W^{(k+r/p)}, v) - \sum_{k=1}^{Q-1} \sum_{r=i+1}^{p} a_{ir}(e_W^{(k-1+r/p)}, v)
\]
\[
= a_i(e_D^{(Q+i/p)}, v) - \sum_{k=0}^{Q} \sum_{r=1}^{i-1} a_{ir}(e_W^{(k+r/p)}, v) - \sum_{k=0}^{Q-1} \sum_{r=i+1}^{p} a_{ir}(e_W^{(k-1+r/p)}, v).
\]
Lemma 5 (Sum of RHS of the adjoint equations over iterations). Let \( 2 \leq M \leq p + 1 \) and \( R = M - 1 \) and \( 0 \leq Q < K \). Then

\[
\left( \sum_{k=0}^{Q} \tau_{R}^{Q}(e_{W}^{(k+R/p)}) \right) - \sum_{k=0}^{Q} \sum_{j=M}^{p} a_{Rj}(e_{W}^{(k+R/p)}, \phi^{[Q+j/p]}) = a_{R}(e_{D}^{(Q+R/p)}, \phi^{[Q+R/p]}) - \sum_{k=0}^{Q} \sum_{i=1}^{R-1} a_{iR}(e_{W}^{(k+i/p)}, \phi^{[Q+R/p]}) - \sum_{k=0}^{Q-1} \sum_{i=M}^{p} a_{iR}(e_{W}^{(k+i/p)}, \phi^{[Q+R/p]}).
\]

(54)

Proof. From the adjoint equation (21) we have

\[
a_{R}(e_{W}^{(k+R/p)}, \phi^{[Q+R/p]}) = \tau_{i}^{Q}(e_{W}^{(k+R/p)}) - \sum_{j=M}^{p} a_{Rj}(e_{W}^{(k+R/p)}, \phi^{[Q+j/p]}). \]

(55)

From Lemma 4

\[
\sum_{k=0}^{Q} a_{R}(e_{W}^{(k+R/p)}, \phi^{[Q+R/p]})
\]

\[
= a_{R}(e_{D}^{(Q+R/p)}, \phi^{[Q+R/p]}) - \sum_{k=0}^{Q} \sum_{i=1}^{R-1} a_{iR}(e_{W}^{(k+i/p)}, \phi^{[Q+R/p]}) - \sum_{k=0}^{Q-1} \sum_{i=M}^{p} a_{iR}(e_{W}^{(k+i/p)}, \phi^{[Q+R/p]}). \]

(56)

Combining (55) and (56) proves the result.

Lemma 6 (Sum of RHS of the adjoint equations over iterations and subdomains). Let \( 1 \leq M \leq p + 1 \) and \( 0 \leq Q < K \). Then we have,

\[
I = \sum_{k=0}^{Q} \sum_{i=1}^{p} \tau_{i}^{Q}(e_{W}^{(k+i/p)}) = \sum_{i=M}^{p} a_{i}(e_{W}^{(Q+i/p)}, \phi^{[Q+(i+1)/p]}) + \sum_{k=0}^{Q} \tau_{i}^{Q}(e_{W}^{(k+i/p)}) - \sum_{k=0}^{Q} \sum_{i=1}^{p} a_{i}(e_{W}^{(Q+i/p)}, \phi^{[Q+(i+1)/p]}) - \sum_{k=0}^{Q-1} \sum_{i=M}^{p} a_{i}(e_{W}^{(Q+i/p)}, \phi^{[Q+(i+1)/p]}) + \sum_{k=0}^{Q-1} \tau_{i}^{Q}(e_{W}^{(k+i/p)}) - \sum_{k=0}^{Q-1} \sum_{i=M}^{p} a_{i}(e_{W}^{(Q+i/p)}, \phi^{[Q+i+1/p]}).
\]

(57)

Proof. The proof is by induction on \( M \).

[1] For \( M = p + 1 \) the right-hand side of (57) is simply \( I \).

[II] Assume that the expression holds for some \( 2 \leq M \leq p \).

[III] To show the result is true for \( M = p - 1 \), we isolate terms involving \( e_{W}^{(k+(M-1)/p)} \).

\[
I = \sum_{i=0}^{p} a_{i}(e_{W}^{(Q+i/p)}, \phi^{[Q+(i+1)/p]}) + \sum_{k=0}^{Q} \sum_{i=1}^{p} \tau_{i}^{Q}(e_{W}^{(k+i/p)}) - \sum_{k=0}^{Q} \sum_{i=1}^{p} a_{i}(e_{W}^{(Q+i/p)}, \phi^{[Q+(i+1)/p]}) - \sum_{k=0}^{Q-1} \sum_{i=M}^{p} a_{i}(e_{W}^{(Q+i/p)}, \phi^{[Q+i+1/p]}) + \sum_{k=0}^{Q} \tau_{i}^{Q}(e_{W}^{(k+i/p)}) - \sum_{k=0}^{Q-1} \sum_{i=M}^{p} a_{i}(e_{W}^{(Q+i/p)}, \phi^{[Q+i+1/p]})
\]

(58)
Combining (59) with (58)

\[ \sum_{k=0}^{Q} \tau_{M-1}^{Q}(e_{W}^{(k+(M-1)/p)}) - \sum_{k=0}^{Q} \sum_{j=M}^{p} a_{M-1,j}(e_{W}^{(k+(M-1)/p)}, \phi^{(Q+j)/p}) \]

\[ = a_{M-1}(e_{D}^{(Q+(M-1)/p)}, \phi^{(Q+(M-1)/p)}) - \sum_{k=0}^{Q} \sum_{i=1}^{M-2} a_{i,M-1}(e_{W}^{(k+i)/p}, \phi^{(Q+(M-1)/p)}) \]

\[ - \sum_{k=0}^{Q-1} \sum_{i=M}^{p} a_{i,M-1}(e_{W}^{(k+i)/p}, \phi^{(Q+(M-1)/p)}). \]

Combining (59) with (58)

\[ I = \sum_{i=1}^{p} a_{i}(e_{D}^{(Q+i)/p}, \phi^{(Q+i)/p}) + \sum_{k=0}^{Q} \sum_{i=1}^{M-2} \tau_{i}^{Q}(e_{W}^{(k+i)/p}) - \sum_{k=0}^{Q} \sum_{i=1}^{M-2} \sum_{j=M-1}^{p} a_{i,j}(e_{W}^{(k+i)/p}, \phi^{(Q+j)/p}) \]

\[ - \sum_{k=0}^{Q-1} \sum_{i=M}^{p} \sum_{j=M-1}^{i-1} a_{i,j}(e_{W}^{(k+i)/p}, \phi^{(Q+j)/p}). \]

\[ \text{Corollary 1.} \text{ Let } 0 \leq Q < K. \text{ Then we have} \]

\[ \sum_{k=0}^{Q} \sum_{i=1}^{p} \tau_{i}^{Q}(e_{W}^{(k+i)/p}) = \sum_{i=1}^{p} a_{i}(e_{D}^{(Q+i)/p}, \phi^{(Q+i)/p}) + \sum_{k=0}^{Q} \sum_{i=1}^{Q-1} \tau_{i}^{Q-1}(e_{W}^{(k+i)/p}). \]

\[ \text{Proof.} \text{ Set } M = 1 \text{ in Lemma 5 to get,} \]

\[ \sum_{k=0}^{Q} \sum_{i=1}^{p} \tau_{i}^{Q}(e_{W}^{(k+i)/p}) = \sum_{i=1}^{p} a_{i}(e_{D}^{(Q+i)/p}, \phi^{(Q+i)/p}) - \sum_{k=0}^{Q} \sum_{i=2}^{p} \sum_{j=1}^{Q-1} a_{i,j}(e_{W}^{(k+i)/p}, \phi^{(Q+j)/p}) \]

\[ = \sum_{i=1}^{p} a_{i}(e_{D}^{(Q+i)/p}, \phi^{(Q+i)/p}) - \sum_{k=0}^{Q-1} \sum_{i=2}^{p} \tau_{i}^{Q-1}(e_{W}^{(k+i)/p}) \]

\[ = \sum_{i=1}^{p} a_{i}(e_{D}^{(Q+i)/p}, \phi^{(Q+i)/p}) - \sum_{k=0}^{Q-1} \sum_{i=1}^{Q-1} \tau_{i}^{Q-1}(e_{W}^{(k+i)/p}), \]

where we used (22) and noticed that \( \tau_{1}^{Q}(v) = 0 \) for \( Q < K - 1. \)

\[ \text{6.1.3 Proof of Theorem 3.2.2} \]

\[ \text{Proof.} \text{ From Lemma 2 and 22,} \]

\[ (e_{D}^{(K), \psi}) = \sum_{k=0}^{K-1} \sum_{i=1}^{p} \sum_{j=1}^{p} (e_{W}^{(k+i)/p}, \psi_{j})_{i,j} = \sum_{k=0}^{K-1} \sum_{i=1}^{p} \tau_{i}^{K-1}(e_{W}^{(k+i)/p}). \]

Applying Corollary 1 leads to

\[ (e_{D}^{(K), \psi}) = \sum_{i=1}^{p} a_{i}(e_{D}^{(K-1+i)/p}, \phi^{(K-1+i)/p}) - \sum_{k=0}^{K-2} \sum_{i=1}^{p} \tau_{i}^{K-2}(e_{W}^{(k+i)/p}). \]

Repeating application of Corollary 1 leads to

\[ (e_{D}^{(K), \psi}) = \sum_{k=0}^{K-1} \sum_{i=1}^{p} a_{i}(e_{D}^{(k+i)/p}, \phi^{(k+i)/p}). \]

\[ \text{18} \]
Now,
\[ a_i(e_{D}^{(k+i)/p}, \phi^{[k+i]/p}) = a_i(u^{(k+i)/p} - U^{(k+i)/p}, \phi^{[k+i]/p}) = a_i(u^{(k+i)/p} - \overline{U}^{(k+i)/p}, \phi^{[k+i]/p}) \]
\[ = l_i(\phi^{[k+i]/p}) - a_i(\overline{U}^{(k+i)/p}, \phi^{[k+i]/p}) = R_i(\overline{U}^{(k+i)/p}, \phi^{[k+i]/p}). \]  
(66)

Combining (65) and (66) leads to
\[ (\psi, u^{(K)} - U^{(K)}) = \sum_{k=0}^{K-1} \sum_{i=1}^{p} R_i(\overline{U}^{(k+i)/p}, \phi^{[k+i]/p}). \]  
(67)

The discrete equivalent of (8) is
\[ R_i(\overline{U}^{(k+i)/p}, v) = l_i(v) - a_i(\overline{U}^{(k+i)/p}, v) \quad \forall v \in V_{i,h,0} \]  
(68)

This equation is often referred to as Galerkin orthogonality. Substituting \( v = \pi \phi^{[k+i]/p} \in V_{i,h,0} \) in (68) and subtracting the result from (67) completes the proof.

6.2 Details of analysis of additive Schwarz algorithm

6.2.1 Reformulation of the algorithm

Similar to the multiplicative case in §6.1, the basic additive algorithm 2 is not amenable to adjoint based analysis since the affine solution space \( H_{D,0}^{1}(\Omega_i) \) changes at every iteration. We reformulate the algorithm by again using a standard lifting technique to account for this. We set
\[ \tilde{w}_{i}^{(k+1)} = w_{i}^{(k+1)} + u^{(k)} \quad \text{on } \Omega_i \]  
(69)

where now \( w_{i}^{(k+1)} \in H_{0}^{1}(\Omega_i) \). This results in Algorithm 5.

Algorithm 5 Reformulated overlapping additive Schwarz

Given \( u^{(0)} \) defined on \( \Omega \).
for \( k = 0, 1, 2, \ldots, K - 1 \) do
   for \( i = 1, 2, \ldots, p \) do
      Find \( w_{i}^{(k+1)} \in H_{0}^{1}(\Omega_i) \) such that
      \[ a_i(w_{i}^{(k+1)}, v) = l_i(v) - a_i(u^{(k)}, v) \quad \forall v \in H_{0}^{1}(\Omega_i). \]  
(70)

   Let \( \tilde{\Pi} w_{i}^{(k+1)} = \begin{cases} w_{i}^{(k+1)} & \text{on } \overline{\Omega}_i \\ 0 & \text{on } \Omega \setminus \overline{\Omega}_i \end{cases} \)

   Let
   \[ u^{(k+1)} = u^{(k)} + \tau \left( \sum_{i=1}^{p} \tilde{\Pi} w_{i}^{(k+1)} \right). \]  
(71)
end for
end for

There is an equivalent reformulation of the discrete Algorithm 5 as Algorithm 2 involving finite dimensional FEM spaces. We denote the unknown solutions in this case as \( W^{(k)} \) belonging to the spaces \( V_{i,h,0} \subset H_{0}^{1}(\Omega_i) \). Note that the solutions \( W^{(k)} \) are devices for the analysis of the algorithm and are not computed in practice.

To distinguish between different solutions (true, analytical, discrete) we use the notation in Table 15.
Lemma 8 (Bilinear form with global discretization errors). For any $v \in V_i$ we have,

$$ a_i(e_D^{(k)}, v) = \tau \sum_{m=1}^{k} \sum_{j=1}^{p} a_{ij}(e_{W_i}^{(m)}, v). $$

Table 15: Additive Schwarz: notation for different solutions and their spaces.

| Notation | Formula | Space | Meaning |
|----------|---------|-------|---------|
| $u$      | $u^{(k)}$ | $H_0^1(\Omega)$ | True solution |
| $u^{(k)}$ | $U^{(k)}$ | $H_0^1(\Omega_i)$ | Global analytic solution at iteration $k$ |
| $\tilde{u}_i^{(k)}$ | $\tilde{U}_i^{(k)}$ | $V_{i,h}$ | Global discrete solution at iteration $k$ |
| $w_i^{(k)}$ | $W_i^{(k)}$ | $H_0^1(\Omega_i)$ | Analytic solutions on $\Omega_i$ at iteration $k$ |
| $\tilde{e}_i^{(k)}$ | $\tilde{e}_i^{(k)}$ | $V_{i,h,0}$ | Discrete solutions on $\Omega_i$ at iteration $k$ |
| $e_i^{(k)}$ | $e_i^{(k)}$ | $H_0^1(\Omega_i)$ | Analytic solutions on $\Omega_i$ with homogeneous bcs at iteration $k$ |
| $e_i^{(k)}$ | $w_i^{(k)} - W_i^{(k)}$ | $H_0^1(\Omega_i)$ | Discrete solutions on $\Omega_i$ with homogeneous bcs at iteration $k$ |

6.2.2 Technical lemmas

Let $e_W^{(k)} = u^{(k)} - W^{(k)}$. By (71) we have

$$ e_D^{(k)} = e_D^{(k-1)} + \tau \sum_{i=1}^{p} e_{W_i}^{(k)} $$  (72)

We apply lemma 1 to arrive at,

$$ (e_D^{(k)}, \psi) = (e_D^{(k)} \sum_{i=1}^{p} \chi_i \psi) = \sum_{i=1}^{p} (e_D^{(k)}, \psi_i) $$  (73)

**Lemma 7** (Error in QoI in terms of discretization errors with homogeneous boundary conditions). The discretization error in the QoI is,

$$ (e_D^{K}, \psi) = \tau \sum_{k=1}^{K} \sum_{i=1}^{p} \sum_{j=1}^{p} (e_{W_i}^{(k)}, \psi_j). $$  (74)

**Proof.** For fixed $j$

$$ (e_D^{K}, \psi_j) = (e_D^{K-1}, \psi_j) + \tau \sum_{i=1}^{p} (\tilde{E} e_{W_i}^{(K)}, \psi_j), $$  (75)

where $\tilde{E}$ This is a recursive relation involving $\tilde{e}^{(K)}$. Unrolling the recursion leads to,

$$ = \tau \sum_{k=1}^{K} \sum_{i=1}^{p} (\tilde{E} e_{W_i}^{(k)}, \psi_j). $$  (76)

Summing over all $j = 1, \ldots, p$,

$$ (\tilde{e}^{(K)}, \psi) = \tau \sum_{k=1}^{K} \sum_{i=1}^{p} \sum_{j=1}^{p} (\tilde{E} e_{W_i}^{(k)}, \psi_j), $$  (77)

since all inner products are over subsets of subdomain $i$ where $\tilde{E}$ is the identity.

**Lemma 8** (Bilinear form with global discretization errors). For any $v \in V_i$ we have,

$$ a_i(e_D^{(k)}, v) = \tau \sum_{m=1}^{k} \sum_{j=1}^{p} a_{ij}(e_{W_i}^{(m)}, v). $$  (78)
Proof. By (72) we have,
\[ a_i(e_D^{(k)},v) = \sum_{j=1}^{p} a_{ij}(e_{W,j}^{(k)},v) + \tau \sum_{j=1}^{p} a_{ij}(e_{W,j}^{(k)},v) \]
(79)
and using the fact that \( e_W = I \). This is a recursive relation involving \( a_i(e_D^{(k)},v) \). Unrolling this recursion and using the fact that \( e_D^{(k)} = 0 \) proves the result.

Lemma 9 (Bilinear form with discretization errors with homogeneous boundary conditions and adjoint solutions).
\[ a_i(e_W^{(k)},\phi_i^{[k]}) = R_i(U_i^{(k)},\phi_i^{[k]}) - \tau \sum_{m=1}^{p} \sum_{j=1}^{p} a_{ij}(e_{W,j}^{(m)},\phi_i^{[k]}) \]
(80)

Proof. By definition of \( e_W^{(k)} \),
\[ a_i(e_W^{(k)},\phi_i^{[k]}) = a_i(w_i^{(k)},\phi_i^{[k]}) - a_i(U_i^{(k)},\phi_i^{[k]}) \]
(81)
Using (69) followed by (70) and definition of \( e_D^{(k)} \),
\[ a_i(e_W^{(k)},\phi_i^{[k]}) = a_i(w_i^{(k)},\phi_i^{[k]}) - a_i(U_i^{(k)},\phi_i^{[k]}) - a_i(U_i^{(k-1)},\phi_i^{[k]}) + a_i(U_i^{(k-1)},\phi_i^{[k]}) \]
(82)
By Lemma 8,
\[ a_i(e_W^{(k)},\phi_i^{[k]}) = R_i(U_i^{(k)},\phi_i^{[k]}) - \tau \sum_{m=1}^{p} \sum_{j=1}^{p} a_{ij}(e_{W,j}^{(m)},\phi_i^{[k]}) \]
(83)

6.2.3 Proof of Theorem 4

Proof. By (24),
\[ (\psi,e_D^{(K)}) = \sum_{k=1}^{K} \sum_{i=1}^{p} \sum_{j=1}^{p} a_{ij}(e_{W,i}^{(k)},\phi_i^{[k]}) = \sum_{k=1}^{K} \sum_{i=1}^{p} \sum_{j=1}^{p} a_{ij}(e_{W,i}^{(k)},\phi_i^{[k]}) + \tau \sum_{j=1}^{p} \sum_{i=k+1}^{K} a_{ij}(e_{W,i}^{(k)},\phi_j^{[l]}) \]
(84)
By Lemma 9,
\[ (\psi,e_D^{(K)}) = \sum_{k=1}^{K} \sum_{i=1}^{p} \sum_{j=1}^{p} a_{ij}(e_{W,i}^{(k)},\phi_i^{[k]}) - \tau \sum_{m=1}^{p} \sum_{j=1}^{p} a_{ij}(e_{W,j}^{(m)},\phi_i^{[k]}) + \tau \sum_{j=1}^{p} \sum_{i=k+1}^{K} a_{ij}(e_{W,i}^{(k)},\phi_j^{[l]}) \]
(85)
Application of Galerkin orthogonality, similar to its use in the proof in 6.1.3 leads to,
\[ (\psi,e_D^{(K)}) = \sum_{k=1}^{K} \sum_{i=1}^{p} \sum_{j=1}^{p} a_{ij}(e_{W,i}^{(k)},\phi_i^{[k]}) - \pi(\phi_i^{[k]}) - \tau \sum_{m=1}^{p} \sum_{j=1}^{p} a_{ij}(e_{W,j}^{(m)},\phi_i^{[k]}) + \tau \sum_{j=1}^{p} \sum_{i=k+1}^{K} a_{ij}(e_{W,i}^{(k)},\phi_j^{[l]}) \]
(86)
The result follows if
\[ \sum_{k=1}^{K} \sum_{j=1}^{p} \sum_{m=1}^{p} a_{ij}(e_{W,i}^{(k)},\phi_j^{[l]}) = \sum_{k=1}^{K} \sum_{i=1}^{p} \sum_{j=1}^{p} \sum_{l=k+1}^{K} a_{ij}(e_{W,i}^{(k)},\phi_j^{[l]}) \]
(87)
where we interchanged the \( i \) and \( j \) loop indices on the left hand side. This follows if,
\[
\sum_{k=1}^{K} \sum_{m=1}^{k-1} a_{ij} \langle e_{W,i}^{\{m\}}, \phi_j^{\{k\}} \rangle = \sum_{k=1}^{K} \sum_{l=k+1}^{K} a_{ij} \langle e_{W,i}^{\{k\}}, \phi_j^{\{l\}} \rangle .
\] (88)

To see why this is true, let \( A \) be a \( K \times K \) strictly lower triangular matrix where the non-zero entries are given by \( A_{k,m} = a_{ij} \langle e_{W,i}^{\{m\}}, \phi_j^{\{k\}} \rangle \) for \( m < k \). Then the left hand side of (88) is the sum of the entries of \( A \) by first summing each row while the right hand side of (88) is the sum of the entries of \( A \) by first summing each column.

\( \Box \)

7 Conclusions and future directions

We have developed an adjoint based \( a \ posteriori \) error analysis to evaluate the separate discretization and iteration errors for a given quantity of interest when solving boundary value problems using overlapping domain decomposition employing either multiplicative or additive Schwarz iteration. The additional expense of formulating and solving the necessary sequence of adjoint problems both recommends and enables a two stage approach to constructing efficient solution strategies. In this approach a “stage one” solution is computed on a relatively coarse discretization employing a small number of iterations or small overlap between subdomains. The error in the quantity of interest is determined for the stage one solution and the balance of discretization and iteration errors, and the distribution of discretization error between subdomains is determined. These guide the solution strategy for a more accurate “stage two” solution in terms of the localized refinement of the finite element mesh and the choices of overlap and number of iterations.

The adjoint based analysis in this article has focused exclusively on linear problems. There is no unique definition of an adjoint operator to a nonlinear differential equation, but a common choice useful for various kinds of analysis ([?]) is based on linearization. Considering equation (1) again, where \( L \) is now a nonlinear operator and setting \( z = su + (1 - s)U \), we define the linearized adjoint operator to be
\[
(DL)^* = \left[ \int_0^1 \frac{\partial L}{\partial u} \bigg|_{z} \, ds \right]^*,
\] (89)
and the corresponding linearized adjoint problem to be
\[
(DL)^* \phi = \psi. \tag{90}
\]

Formally, we use the solution of (90) in the \( a \ posteriori \) error analysis to obtain (5), but in practice, we linearize around the numerical solution. The resulting estimate can be shown to converge to the true estimate in the limit of refined discretization [?] and yields robustly accurate error estimates. A consideration of nonlinear problems is therefore an obvious and relatively immediate extension of this work.

A more serious extension is to address initial boundary value problems. To begin, we will employ simple implicit time integrators. We then aim to combine the current analysis with earlier work on parallel methods for initial value problems [10], to develop an \( a \ posteriori \) analysis for a method that is parallel in both space and time. Once again we will adopt a two stage solution approach, using the distribution of various sources of error estimated from an initial coarse solve to inform the discretization choices for a second “production” computation.

We will also analyse non-overlapping domain decomposition such as FETI [17, 16] and BDDC [15, 27] methods by extending work on Lions domain decomposition [8] and mortar elements [2, 3] to develop distinct estimates of the errors arising on domain interiors and interfaces. This is particularly appropriate when the quantity of interest, for example a flux, is defined on the boundary between two or more domains.

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