



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 high performance computers. We develop an adjoint-based a posteriori error analysis for both multiplicative and additive overlapping Schwarz domain decomposition methods. The numerical error in a user-specified functional of the solution (quantity of interest) is decomposed into contributions that arise as a result of the finite iteration between the subdomains and from the spatial discretization. The spatial discretization contribution is further decomposed into contributions arising from each subdomain. This decomposition of the numerical error is used to construct a two stage solution strategy that efficiently reduces the error in the quantity of interest by adjusting the relative contributions to the error.

Keywords Schwarz overlapping domain decomposition · A posteriori error estimation · Adaptive computation

Mathematics Subject Classification 65N15 · 65N50 · 65N55 · 68W10

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1 Introduction

We derive and implement an adjoint-based a posteriori error analysis for overlapping domain decomposition methods for elliptic 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 [31,37]. Recently DDMs have seen increased use in the context of distributed and parallel computing [30,35,38–40]. In this article, we follow the presentation in [35].

In overlapping DDMs, each subdomain has a non-empty intersection with at least one other subdomain and typically state information is exchanged between the subdomains. The theoretical properties of the multiplicative Schwarz method and some of its variants were studied in [33]. The variant of this method suitable for parallel computing, called the additive Schwarz method, was introduced in [19]. Non-overlapping DDMs, in which the subdomains have empty intersection and state and derivative information is exchanged through their common interfaces, is an alternative approach [32].

Adjoint-based a posteriori error analysis for systems of ordinary and partial differential equations has an extensive history [3,4,20,21,26,27], and has been applied to a wide range of applications and numerical methods [1,2,8,10–12,14–18,29]. Adjoint-based a posteriori error analysis classically considers a differential equation

$$L(u(\mathbf{x}, t)) = g(\mathbf{x}, t), \quad (1)$$

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

$$Q(u) = (u, \psi), \quad (2)$$

where (\cdot, \cdot) denotes the L_2 inner product and the function ψ 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, $(u - U, \psi)$. The relation between the residual and the error is derived from solving an adjoint problem.

For linear problems, the adjoint operator $\mathcal{L}^* : Y^* \rightarrow X^*$ of a linear operator $\mathcal{L} : X \rightarrow Y$ between Banach spaces X, Y with dual spaces X^*, Y^* is defined by the bilinear identity

$$\langle \mathcal{L}x, y^* \rangle_Y = \langle x, \mathcal{L}^*y^* \rangle_{X^*}, \quad x \in X, y^* \in Y^*, \quad (3)$$

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

$$L^* \phi = \psi. \quad (4)$$

This yields the error estimate,

$$\text{Error in the QoI} = (u - U, \psi) = (R(U), \phi). \quad (5)$$

We estimate the numerical error in the quantity of interest by numerically solving the adjoint problem (4), computing the residual, and evaluating (5).

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 for which 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 the adjoint of the overall problem (4). The correct choice of adjoint and residuals also enables a decomposition of the total error into 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], in an analysis of a multirate iterative solver for ordinary differential equations in [23], and in an analysis of an iterative multi-discretization method for reaction–diffusion systems in [13]. An a posteriori error analysis for non-overlapping DDM is carried out in [8]. To the best of our knowledge, an a posteriori error analysis for overlapping DDMs has not been performed. Domain decomposition methods may converge slowly and iterating to convergence not only wasteful, but can be prohibitively expensive, thus independent estimates of discretization and iterative error are of considerable value.

Adjoint-based a posteriori error estimates can provide useful information for designing efficient adaptive solution strategies. During the first “pre-processing” step (stage 1), 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 “production level” (stage 2) computation. This strategy is described in earlier work on blockwise adaptivity [6,29] and in [11].

Other a posteriori approaches have been developed for providing upper and lower bounds on the iterative (algebraic) and discretization errors when solving a finite element scheme with an iterative method, and these bounds been used to drive adaptive solution strategies [28,36]. Upper and lower bounds on the discretization errors are obtained through the solution of multiple localized “patch” problems. Bounds on the iteration error are obtained through a consideration of the differences between solutions

after a given number of iterations and the solutions obtained after an additional number of iterations.

Accurate error estimates are also an essential component for the accurate quantification of uncertainty when the problem specification is in doubt, either through uncertainty in parameter values, the computational domain or the model description itself. The numerical error introduced in stochastic computations varies as each of these components defining the problem is varied, and examples of each are described in [5, 8, 14, 25, 25]. The ability to capture the subtle interplay between different sources of error and their potential for cancellation is essential in all cases. These features can be obscured by considering sources of error in isolation and by taking bounds.

We introduce the multiplicative and additive Schwarz overlapping domain decomposition methods in Sect. 2. We present the a posteriori error analysis in Sect. 3. Examples are provided for multiplicative Schwarz in Sect. 4 and for additive Schwarz in Sect. 5. Details of the analysis appear in Sect. 6. A discussion and future research directions appear in Sect. 7.

2 Overlapping Schwarz domain decomposition

Assume that we have p overlapping subdomains $\Omega_1, \dots, \Omega_p$ on a domain Ω , such that for any Ω_i , there exists a Ω_j , $i \neq j$, for which $\Omega_i \cap \Omega_j \neq \emptyset$ and $\cup_i \Omega_i = \Omega$. We consider overlapping domain decomposition algorithms for partial differential equations (PDEs) given in the weak form: find $u \in V$ such that

$$a(u, v) = l(v) \quad \forall v \in V. \quad (6)$$

Here $a(\cdot, \cdot)$ is the standard bilinear form over Ω arising from integration by parts of the PDE operator, $l(\cdot)$ is the linear functional arising from the right-hand-side of the PDE and V is an appropriate function space. Such PDEs model a variety of physical phenomena ranging from biomolecular simulation and diffusive processes, to Darcy flow and linear elasticity. We use $L_2(\Omega)$ to denote the space of square integrable functions, $H^1(\Omega)$ for functions having a $L_2(\Omega)$ derivative and $H_0^1(\Omega)$ as the subspace of $H^1(\Omega)$ of functions satisfying homogeneous Dirichlet boundary conditions. We let (\cdot, \cdot) and $(\cdot, \cdot)_{ij}$ represent the $L_2(\Omega)$ and $L_2(\Omega_i \cap \Omega_j)$ inner products respectively.

To be specific, we consider the weak form of a second-order linear elliptic PDE problem: find $u \in V = H_0^1(\Omega)$ such that

$$a(u, v) = l(v) \quad \forall v \in H_0^1(\Omega). \quad (7)$$

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 $a(\cdot, \cdot)$ to Ω_i and $a_{ij}(\cdot, \cdot)$ the restriction of $a(\cdot, \cdot)$ to $\Omega_i \cap \Omega_j$. Similarly, we let $l_i(\cdot)$ be the restriction of $l(\cdot)$ to Ω_i .

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

$$Q(u) = (\psi, u), \quad (8)$$

where $\psi \in L_2(\Omega)$.

2.1 Multiplicative Schwarz overlapping domain decomposition

Defining $H_{D_k}^1(\Omega_i) \equiv \{v \in H^1(\Omega_i) \mid v = u^{[k+(i-1)/p]} \text{ on } \partial\Omega_i\}$, we present the multiplicative Schwarz method in Algorithm 1, for K iterations over the p subdomains.

Algorithm 1 Overlapping multiplicative Schwarz domain decomposition

Given $u^{[0]}$ defined on Ω
for $k = 0, 1, 2, \dots, K - 1$ **do**
 for $i = 1, 2, \dots, p$ **do**
 Find $\tilde{u}^{[k+i/p]} \in H_{D_k}^1(\Omega_i)$ such that

$$a_i(\tilde{u}^{[k+i/p]}, v) = l_i(v), \quad \forall v \in H_0^1(\Omega_i). \quad (9)$$

Let

$$u^{[k+i/p]} = \begin{cases} \tilde{u}^{[k+i/p]}, & \text{on } \overline{\Omega_i}, \\ u^{[k+(i-1)/p]}, & \text{on } \Omega \setminus \overline{\Omega_i}. \end{cases} \quad (10)$$

end for
end for

2.2 Additive Schwarz overlapping domain decomposition

The additive Schwarz solution method is given in Algorithm 2 with $H_{D_k}^1(\Omega_i) \equiv \{v \in H_D^1(\Omega_i) \mid v = u^{[k]} \text{ on } \partial\Omega_i\}$. The Richardson parameter τ , is needed to ensure that the iteration converges [35].

Algorithm 2 Overlapping additive Schwarz domain decomposition

Given $u^{[0]}$ defined on Ω
for $k = 0, 1, 2, \dots, K - 1$ **do**
 for $i = 1, 2, \dots, p$ **do**
 Find $\tilde{u}_i^{[k]} \in H_{D_k}^1(\Omega_i)$ such that

$$a_i(\tilde{u}_i^{[k+1]}, v) = l_i(v), \quad \forall v \in H_0^1(\Omega_i). \quad (11)$$

Let

$$u^{[k+1]} = (1 - \tau p)u^{[k]} + \tau \left(\sum_{i=1}^p \Pi_i \tilde{u}_i^{[k+1]} \right) \text{ where } \Pi_i \tilde{u}_i^{[k+1]} = \begin{cases} \tilde{u}_i^{[k+1]}, & \text{on } \overline{\Omega_i}, \\ u^{[k]}, & \text{on } \Omega \setminus \overline{\Omega_i}. \end{cases} \quad (12)$$

end for
end for

2.3 Finite element discretizations

We let $\mathcal{T}_h = \{T_m\}_{m=1}^M$ denote a quasi-regular triangulation of Ω in to non-overlapping elements T_m such that no node of one element T_i intersects the interior of an edge of another element T_j , i.e., there are no hanging nodes, and $\Omega = \cup_m T_m$. Moreover, the triangulation is consistent with the domain decomposition in the sense that if $T_i \cap \Omega_j \neq \emptyset$ then $T_i \subset \Omega_j$. The discretization of the overlapping domain decomposition approximation substitutes finite dimensional spaces $V_{i,h}^k$ for $H_{D_k}^1(\Omega_i)$ and $V_{i,h,0}$ for $H_0^1(\Omega_i)$ in Algorithm 1, where $V_{i,h}^k$ and $V_{i,h,0}$ refer to the standard finite element spaces consisting space of continuous piecewise polynomial functions on $\mathcal{T}_{h,i} = \mathcal{T}_h|_{\Omega_i}$. Additionally, $V_h \subset H_0^1(\Omega)$ is the finite element space consisting of continuous piecewise polynomial functions with respect to \mathcal{T}_h .

We represent the global discrete solutions as $U^{\{k+i/p\}}$ (resp. $U_i^{\{k\}}$) belonging to the space V_h and the local discrete solutions as $\tilde{U}^{\{k+i/p\}}$ (resp. $\tilde{U}_i^{\{k\}}$) belonging to the space $V_{i,h,0}$ for the multiplicative (resp. additive) Schwarz methods. For simplicity we assume that $U^{\{0\}} = u^{\{0\}}$. For both algorithms, the global continuum, (resp. discrete), solution after k iterations is represented as $u^{\{k\}}$, (resp. $U^{\{k\}}$).

3 A posteriori analysis for the finite element approximation computed using Schwarz algorithms

We derive a representation formula for the error in the QoI, $Q(u) - Q(U^{\{K\}}) = (\psi, u - U^{\{K\}})$, that is computed from the discrete solution of the multiplicative or additive domain decomposition method after K iterations.

3.1 The total error and its components

We first consider the total numerical error, and then its decomposition into discretization and iteration error components.

3.1.1 The total error

We define the *global* adjoint, $\phi \in H_0^1(\Omega)$, such that

$$a(v, \phi) = (\psi, v), \quad \forall v \in H_0^1(\Omega). \quad (13)$$

Theorem 1 (Total error representation) *The error in the QoI for the discretized multiplicative or additive Schwarz algorithm after K iterations is given by*

$$(u - U^{\{K\}}, \psi) = R(U^{\{K\}}, \phi), \quad (14)$$

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., [20]. Unfortunately, it does not capture the structure of the differential operator corresponding to the Schwarz domain decomposition, which is reflected in the lack of Galerkin orthogonality in the expression. Performing Schwarz domain decomposition with a finite number of iterations defines a differential operator which is different than the differential operator associated with the original PDE (7). The numerical solution $U^{[K]}$ is a solution to the discretization of this modified operator. We carry out an analysis by decomposing the error into two contributions: iterative and discretization errors. For implementation purposes we note that the global adjoint ϕ is solved using a higher order finite element scheme. The global adjoint may be approximated by a Schwarz domain decomposition method provided sufficient iterations are performed, or the overlap is sufficiently large that the iteration error is negligible.

3.1.2 Discretization and iteration errors

We decompose the total error as

$$u - U^{[K]} = \underbrace{u - u^{[K]}}_{\text{Iteration Error}} + \underbrace{u^{[K]} - U^{[K]}}_{\text{Discretization Error}} = e_I^{[K]} + e_D^{[K]}, \quad (15)$$

where $e_I^{[k]} = u - u^{[k]}$, $e_D^{[k]} = u^{[k]} - U^{[k]}$ and $e_D^{[0]} = 0$. The iteration error quantifies 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 (K) iterations. The discretization error arises from the discretization of the modified differential operator.

Theorem 2 (Iteration error representation) *We have*

$$(u - u^{[K]}, \psi) = R(U^{[K]}, \phi) - (\psi, u^{[K]} - U^{[K]}). \quad (16)$$

Proof This follows by combining (14) and (15). \square

The analysis involves partitioning of the QoI data over subdomains by a partition of unity. Similar ideas were used in [24]. Let $\{\chi_i\}_{i=1}^p$ be a partition of unity such that

$$\psi_i = \chi_i \psi, \quad (17)$$

and $\psi_i = 0$ on $\Omega \setminus \Omega_i$. The partition of unity localizes the QoI data to the subdomains. Let $d_i(x)$ denote the distance function

$$d_i(x) = \begin{cases} \text{dist}(x, B^{(i)}), & \text{if } x \in \overline{\Omega}_i \\ 0, & \text{if } x \notin \overline{\Omega}_i, \end{cases} \quad (18)$$

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

$$\chi_i(x) = \frac{d_i(x)}{\sum_{j=1}^p d_j(x)}. \quad (19)$$

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

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

$$\left(e_D^{\{k\}}, \psi\right) = \sum_{i=1}^p \left(e_D^{\{k\}}, \psi_i\right)_{ii}. \quad (20)$$

Proof This follows directly from the definition of the partition of unity in (17),

$$\left(e_D^{\{k\}}, \psi\right) = \left(e_D^{\{k\}}, \sum_{i=1}^p \chi_i \psi\right) = \sum_{i=1}^p \left(e_D^{\{k\}}, \psi_i\right)_{ii}.$$

□

3.1.3 Weak residuals

We define the subdomain weak residual for a function s , such that

$$R_i(s, v) = l_i(v) - a_i(s, v), \quad \forall v \in H_0^1(\Omega_i), \quad (21)$$

for $i = 1, 2, \dots, p$.

3.2 A posteriori error analysis of discretization error for multiplicative Schwarz

In this section, we derive a representation of the discretization error, $(\psi, u^{\{K\}} - U^{\{K\}})$, for the multiplicative Schwarz method.

3.2.1 Adjoint problems

Define solutions $\phi^{[k+i/p]} \in H_0^1(\Omega_i)$ of the adjoint problems,

$$\begin{cases} a_p(v, \phi^{[Q+i/p]}) = \tau_p^Q(v), & \forall v \in H_0^1(\Omega_p), \\ a_i(v, \phi^{[Q+i/p]}) = \tau_i^Q(v) - \sum_{j=i+1}^p a_{ij}(v, \phi^{[Q+j/p]}), & 1 \leq i < p, \quad \forall v \in H_0^1(\Omega_i), \end{cases} \quad (22)$$

where

$$\tau_i^Q(v) = \begin{cases} \sum_{j=1}^p (v, \psi_j)_{ij}, & Q = K - 1, \\ -\sum_{j=1}^p a_{ij}(v, \phi^{[Q+1+j/p]}), & 0 \leq Q < K - 1. \end{cases} \quad (23)$$

The right hand side of (22) captures not only the residuals corresponding to 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 $-\sum_{j=1}^{i-1} a_{ij} (v, \phi^{[Q+1+j/p]}) - \sum_{j=i+1}^p a_{ij} (v, \phi^{[Q+j/p]})$). The adjoint problems (22) have the same sequential nature of subdomains solves as the multiplicative Schwarz Algorithm 1, but note that these are defined backwards from K , $K-1+(p-1)/p$, $K-1+(p-2)/p, \dots, 1$.

3.2.2 Discretization error

Theorem 3 (Discretization error for multiplicative Schwarz) *We have*

$$(\psi, u^{[K]} - U^{[K]}) = \sum_{k=0}^{K-1} \sum_{i=1}^p R_i \left(\tilde{U}^{[k+i/p]}, \phi^{[k+i/p]} - \pi_i \phi^{[k+i/p]} \right), \quad (24)$$

where $\pi_i v$ is an arbitrary (e.g. L_2 , nodal etc.) projection of $v \in H_0^1(\Omega_i)$ in $V_{i,h,0}$.

The proof of Theorem 3 is presented as a sequence of lemmas in Sect. 6.2. The term $(\phi^{[k+i/p]} - \pi_i \phi^{[k+i/p]})$ arises from the use of Galerkin orthogonality, or the fact that the residual of the discrete solution is zero on the finite dimensional space $V_{i,h,0}$. This reflects the fact that $\tilde{U}^{[k+i/p]}$ is the discrete approximation to $u^{[k+i/p]}$, not to u .

3.3 A posteriori analysis of the discretization error for additive Schwarz

In this section, we derive representation of the discretization error in the QoI obtained from the additive Schwarz method.

3.3.1 Adjoint problems for discretization error

Define $\phi_i^{[k]} \in H_0^1(\Omega_i)$ solutions to the adjoint problems,

$$a_i \left(v, \phi_i^{[k]} \right) = \tau \sum_{j=1}^p \left\{ (\psi_j, v)_{ij} - a_{ij} \left(v, \sum_{l=k+1}^K \phi_j^{[l]} \right) \right\}, \quad \forall v \in H_0^1(\Omega_i). \quad (25)$$

For a fixed k , the adjoint problems (25) are independent for each i , so $\phi_i^{[k]}$ may be computed backwards from K , $K-1$, $K-2, \dots, 1$ in parallel analogous to the solution strategy in the additive Schwarz Algorithm 2. We also note that for implementation purposes $\sum_{l=k+1}^K \phi_j^{[l]}$ involves a sum of the vectors, $\sum_{l=k+2}^K \phi_j^{[l]}$ (computed earlier) and $\phi_j^{[k+1]}$.

3.3.2 Discretization error

Theorem 4 (Discretization error for additive Schwarz) *We have*

$$\left(\psi, e_D^{\{K\}}\right) = \left(\psi, u^{\{K\}} - U^{\{K\}}\right) = \sum_{k=1}^K \sum_{i=1}^p R_i \left(\tilde{U}_i^{\{k\}}, \phi_i^{\{k\}} - \pi_i \phi_i^{\{k\}}\right). \quad (26)$$

The proof of Theorem 4 is presented as a sequence of lemmas in Sect. 6.3.

3.4 Solution algorithms

The full algorithm for a posteriori error estimation for overlapping multiplicative/additive Schwarz domain decomposition is provided in Algorithm 3. We also sketch a two stage procedure in Algorithm 4. The preceding error analysis provides subdomain-by-subdomain contributions to the discretization error and a range of refinement strategies are possible; see Sect. 4.5.1 for a concrete example. Iteration error can be reduced either by increasing the number of iterations or by increasing the size of the overlap regions. An example of this is given in Sect. 4.5.2. Which of these two approaches is preferable cannot be determined by our current analysis. Further, significant grid refinement may require a new division of the computational domain into the same number of subdomains (p) or the addition of further subdomains. Since the accuracy of the error estimates is our primary concern, only the simplest strategies are implemented here.

Algorithm 3 Adjoint-based a posteriori error estimation for overlapping DDMs

```

procedure ERROR ESTIMATION OVERLAPPING DDMs(mesh, p, K, mode)
  for k = 0, 1, 2, ..., K - 1 do
    for i = 1, 2, ..., p do
      Solve primal problem on subdomain i                                (see (9)/(11))
      Combine to construct a global solution                             (see (10)/(12))
    end for
  end for
  if mode == 0 then Return (solution)
  end if
  if mode == 1 then
    for k = K - 1, K - 2, ..., 0 do
      for i = p, p - 1, ..., 1 do
        Approximate solution of adjoint problem on subdomain i        (see (22)/(25))
        Compute adjoint weighted residuals and accumulate error contributions (see (24)/(26))
      end for
    end for
    Approximate solution of global adjoint problem                      (see (13))
    Estimate total error                                                  (see (14))
    Estimate iteration error                                              (see (16))
    Return (solution, total error, discretization error, iteration error)
  end if
end procedure

```

Algorithm 4 Two stage procedure

Call procedure ERROR ESTIMATION OVERLAPPING DDMS(*mesh1*, p_1 , K_1 , 1)

Adapt $mesh1 \rightarrow mesh2$, $p_1 \rightarrow p_2$, $K_1 \rightarrow K_2$

Call procedure ERROR ESTIMATION OVERLAPPING DDMS(*mesh2*, p_2 , K_2 , 0)

4 Numerical examples for multiplicative Schwarz

We provide examples for both multiplicative and additive Schwarz in order to demonstrate the accuracy of the a posteriori error estimate for a range of scenarios, stressing the importance of the ability to distinguish the contributions from discretization and iteration. All adjoint problems are solved on the same mesh as the forward problem using a higher order finite element scheme. Since the adjoint problems are linear, the adjoint problems can be more expensive to solve than the forward problem when the forward problem is also linear, but are generally less expensive to solve when the forward problem is nonlinear. The global adjoint problem was solved using a global discretization.

The initial examples in Sect. 4.2 are chosen to illustrate certain expected behaviors. We expect the discretization error to decrease as the mesh is refined, and the iteration error to decrease as we increase the number of iterations or the degree of overlap. We expect the discretization error to be constant if the mesh is fixed when the number of subdomains is increased, but expect the iteration error to increase. In other words, the discretization error is determined by the mesh, but the iteration error is determined by the number (and disposition) of subdomains, the degree of overlap, and the number of iterations. In Sect. 4.3, we construct a problem where the discretization and iteration errors have opposite signs, and show that iterating with a fixed mesh may result in the overall error initially decreasing as the iteration error decreases, achieving a minimum when the discretization and iteration errors cancel each other, and then increasing (and stabilizing) as the discretization error comes to dominate the total error. For the convection dominated problem in Sect. 4.4, we show how the configuration of the subdomains affects the iteration error, but not the discretization error. Finally in Sect. 4.5 we provide two examples of a two stage strategy in which an accurate error estimate for an initial coarse solution guides the construction of a more accurate “production” calculation. We choose to locally adapt the finite element mesh when the discretization error in a particular subdomain is dominant, and to increase the degree of subdomain overlap when iteration is the leading source of error. “Adaptivity” in the context of iterative methods, requires strategies for addressing both discretization and iteration errors.

4.1 Error estimates and effectivity ratios

We compute approximate adjoint solutions $\Phi^{[k+i/p]} \approx \phi^{[k+i/p]}$, and $\Phi \approx \phi$ and then compute (24) and (14). The resulting error estimates are

$$\eta_D^K \equiv \sum_{k=0}^{K-1} \sum_{i=1}^p R_i(\tilde{U}^{[k+i/p]}, \Phi^{[k+i/p]} - \pi_i \Phi^{[k+i/p]}), \quad (27)$$

and

$$\eta^K \equiv R(U^{\{K\}}, \Phi). \quad (28)$$

One way to measure the performance of an error estimates is the “effectivity ratios”,

$$\gamma = \frac{\eta^K}{(u - U^{\{K\}}, \psi)}, \quad (29)$$

and

$$\gamma_D = \frac{\eta_D^K}{(u^{\{K\}} - U^{\{K\}}, \psi)}. \quad (30)$$

An effectivity ratio close to one indicates that the error estimate is accurate. We also recall that e_I denotes the iteration error. Moreover, we choose π_i to be the trivial projection, that is we set $\pi_i \Phi^{[k+i/p]} = 0$. This is appropriate for the numerical experiments considered in this article in which all mesh elements in a particular subdomain are refined. If the mesh elements in a subdomain are refined based on their localized contribution to error, then a different projection like the nodal projection may be a better choice.

4.2 Poisson’s equation

Consider Poisson’s equation

$$\begin{aligned} -\nabla^2 u &= f, & \text{in } \Omega, \\ u &= 0, & \text{on } \partial\Omega, \end{aligned} \quad (31)$$

in a square domain $\Omega = [0, 1] \times [0, 1]$, where $f(x, y) = 8\pi^2 \sin(2\pi x) \sin(2\pi y)$. The QoI in (8) is specified by

$$\psi = \mathbb{1}_{[.6, .8] \times [.6, .8]}. \quad (32)$$

where $\mathbb{1}_\omega$ is the characteristic function on a domain ω . 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 in a coordinate direction is indicated by β as illustrated by Fig. 2c. The adjoint problems are solved using continuous piecewise quadratic polynomials.

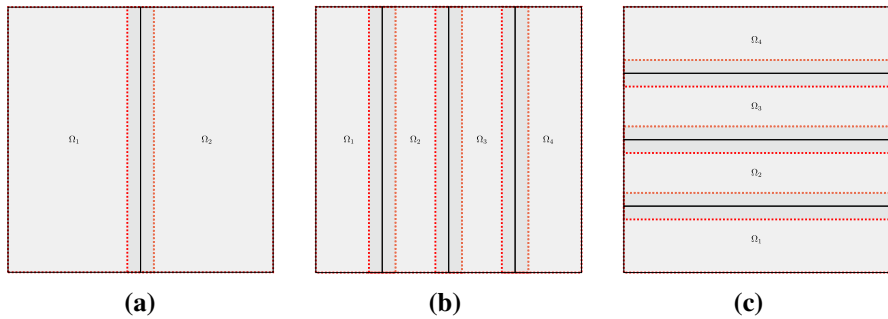


Fig. 1 Overlapping subdomains with $\beta = 0.1$. **a** Two (2×1) subdomains. **b** Four (4×1) subdomains. **c** Four (1×4) subdomains

Table 1 Multiplicative Schwarz for Poisson's equation: 2×1 subdomains

N_x	N_y	β	K	Est. Err.	γ	$e_D^{(K)}$	γ_D	$e_I^{(K)}$
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	2	1.02e-03	9.98E-01	6.56e-04	9.98E-01	3.60e-04
20	20	0.1	4	6.55e-04	9.96E-01	6.26e-04	9.97E-01	2.89e-05
20	20	0.1	6	6.21e-04	9.96e-01	6.19e-04	9.97e-01	2.32e-06
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
80	80	0.1	2	4.01e-04	1.00e+00	4.16e-05	1.00e+00	3.60e-04

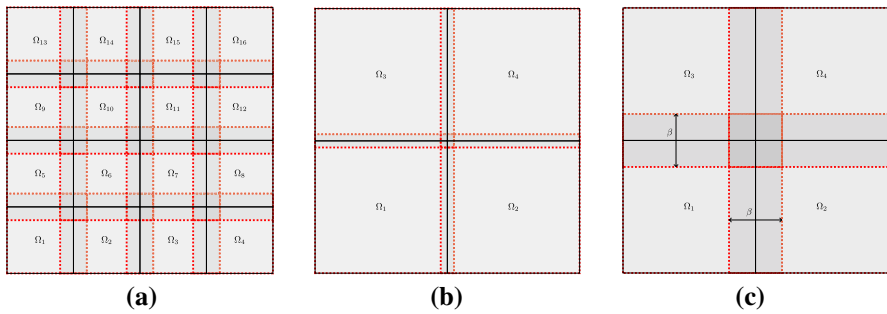
4.2.1 2×1 subdomains

Two overlapping subdomains $\Omega_1 = [0, .6] \times [0, 1]$ and $\Omega_2 = [.4, 1] \times [0, 1]$ are illustrated in Fig. 1a, corresponding to an overlap parameter $\beta = 0.1$. The solid black lines in this figure and in subsequent figures, indicate the center line between overlapping subdomains.

Estimates of the discretization, iteration and total errors, and the corresponding effectivity ratios as we vary the overlap β , number of Schwarz iterations K and number of elements are shown in Table 1. In all cases the effectivity ratios are close to 1.0. The table highlights the sensitivity of the estimates to the different contributions of the 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 $e_D^{(K)}$. The iteration error decreases with increasing number of Schwarz iterations, but the discretization error is largely unaffected when the mesh is fixed. The discretization error decreases when the mesh is refined with a fixed number of iterations, but the iteration error remains essentially constant.

Table 2 Multiplicative Schwarz for Poisson's equation: 4×1 subdomains.

N_x	N_y	β	K	Est. Err.	γ	$e_D^{(K)}$	γ_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	6	6.74e-04	9.96e-01	6.27e-04	9.97e-01	4.67e-05
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
80	80	0.1	2	3.92e-03	1.00e+00	4.39e-05	1.00e+00	3.88e-03

**Fig. 2** **a** Sixteen (4×4) overlapping subdomains with $\beta = 0.1$. **b** Four (2×2) overlapping subdomains with $\beta = 0.05$. **c** Four (2×2) overlapping subdomains with $\beta = 0.2$

4.2.2 4×1 subdomains

The computational domains for $\beta = 0.1$ are shown in Fig. 1b. It is well known that as the number of subdomains increases, the convergence of Schwarz methods decreases, and this is evident by comparing Tables 1 and 2. While the discretization errors of the four subdomain and two subdomain cases are comparable in magnitude, the iteration error $e_I^{(K)}$ is an order of magnitude larger for four subdomains 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 the results in Sect. 4.2.1.

4.2.3 4×4 subdomains

The computational domains for $\beta = 0.1$ and sixteen equally-sized subdomains are configured in a 4×4 grid, see Fig. 2a. The error estimates are quite accurate. The results, shown in Table 3 are qualitatively similar to those in Tables 1 and 2. The iteration error is larger than in the 4×1 case, while the discretization errors are essentially the same in both, which is to be expected since the finite element meshes are the same.

Table 3 Multiplicative Schwarz for Poisson's equation: 4×4 subdomains

N_x	N_y	β	K	Est. Err.	γ	$e_D^{(K)}$	γ_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	6	1.23e-03	9.98e-01	7.07e-04	9.98e-01	5.23e-04
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
80	80	0.1	2	8.26e-03	1.00e+00	6.38e-05	1.00e+00	8.20e-03

4.3 Cancellation of error

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

$$\psi = \mathbb{1}_{[.4, .8] \times [.4, .8]}. \quad (33)$$

for two subdomains and an overlap $\beta = 0.05$. Computational results for an increasing number of Schwarz iterations are shown in Table 4. 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 is 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 -1.6×10^{-4} . The initial iteration error is of order 4.0×10^{-3} and 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, and cancel to produce a total error of 3.0×10^{-5} . For greater than six iterations, the iteration error continues to decrease and now the discretization error dominates the total error. The total error increases to -1.5×10^{-4} after 10 iterations and gradually approaches the (fixed) discretization error as the number of iterations increases further.

4.4 A convection–diffusion problem

Consider the convection–diffusion equation,

$$\begin{aligned} -\nabla^2 u + \mathbf{b} \cdot \nabla u &= f, & \text{in } \Omega, \\ u &= 0, & \text{on } \partial\Omega, \end{aligned} \quad (34)$$

where $\Omega = [0, 1] \times [0, 1]$, $f(x, y) = 1$, and $\mathbf{b} = [-60, 0]$. The effect of the convection is that a perturbation to data on the right affects the solution to the left. For this example,

Table 4 Multiplicative Schwarz for Poisson's equation: 2×1 subdomains, $N_x = N_y = 40$, $\beta = 0.05$

K	Est. Err.	γ	$e_D^{(K)}$	γ_D	$e_I^{(K)}$
1	3.98e-03	1.00e+00	-1.50e-05	9.98e-01	4.00e-03
2	2.07e-03	1.00e+00	-5.95e-05	9.99e-01	2.13e-03
3	1.04e-03	1.00e+00	-9.11e-05	1.00e+00	1.13e-03
4	4.89e-04	1.00e+00	-1.14e-04	1.00e+00	6.03e-04
5	1.91e-04	1.00e+00	-1.30e-04	1.00e+00	3.21e-04
6	2.97e-05	1.01e+00	-1.41e-04	1.00e+00	1.71e-04
7	-5.83e-05	9.96e-01	-1.49e-04	1.00e+00	9.09e-05
8	-1.07e-04	9.98e-01	-1.55e-04	1.00e+00	4.84e-05
9	-1.33e-04	9.98e-01	-1.59e-04	1.00e+00	2.58e-05
10	-1.48e-04	9.98e-01	-1.62e-04	1.00e+00	1.37e-05

we choose the quantity of interest

$$\psi = \mathbb{1}_{[.05, .2] \times [.05, .2]}, \quad (35)$$

concentrated near the bottom left hand corner. The adjoint problems are 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 4×1 configuration

This subdomain configuration is the same as in Fig. 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 direction of information travel from right to left. The iteration error decreases dramatically for $K = 4$ and $K = 6$, and discretization error becomes the dominant error.

4.4.2 1×4 configuration

This subdomain configuration is shown in Fig. 1c. 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 4×1 case. In this scenario, one subdomain contains most of the “domain of influence” for the QoI [24] and hence results in low iteration error, even for $K = 2$. There is again 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.

Table 5 Multiplicative Schwarz for convection–diffusion: $N_x = N_y = 20$, $\beta = 0.1$

K	Est. Err.	γ	$e_D^{(K)}$	γ_D	$e_I^{(K)}$
4×1 configuration					
2	9.76e−03	1.00e+00	−1.54e−04	9.87e−01	9.92e−03
4	−1.15e−04	9.81e−01	−1.42e−04	9.77e−01	2.67e−05
6	−3.54e−04	9.94e−01	−3.54e−04	9.94e−01	4.36e−10
1×4 configuration					
2	8.42e−05	1.03e+00	−3.73e−04	9.94e−01	4.57e−04
4	−3.54e−04	9.94e−01	−3.55e−04	9.94e−01	3.53e−07
6	−3.54e−04	9.94e−01	−3.54e−04	9.94e−01	3.70e−11

4.5 Two stage solution strategy for Poisson’s equation

Adjoint-based a posteriori error estimates can provide useful information for designing efficient two stage strategies for computing approximate solutions, as presented in Algorithm 4 and discussed in Sect. 3.4. First, a preliminary, inexpensive computation is performed on a coarse discretization. The a posteriori error estimate for the “stage 1” solution is computed and the different error contributions determined. A more expensive “stage 2” approximation is computed using numerical parameters chosen to balance the sources of error. We provide two examples of this strategy below. The stage 1 computation for both experiments is run on a 2×2 subdomain configuration as shown in Fig. 2c.

4.5.1 Dominant discretization error

Consider the QoI given by (32). The results on the initial 2×2 subdomain configuration with $N_x = N_y = 10$, $\beta = 0.2$ and $K = 6$ are provided in Table 6. The mesh for this computation is shown in Fig. 3a. The main source of the error is the discretization error $e_D^{(K)}$. 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

$$S_i^K = \sum_{k=0}^{K-1} R_i(\tilde{U}^{[k+i/p]}, \phi^{[k+i/p]} - \pi_i \phi^{[k+i/p]}), \quad i = 1, \dots, p, \quad (36)$$

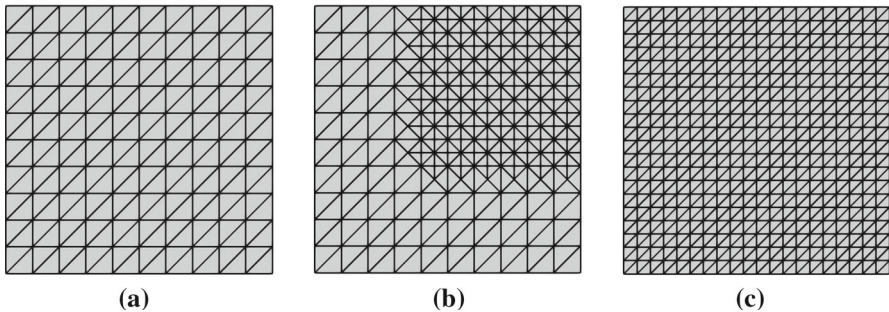
so that the discretization error, (24) may be written as

$$(\psi, u^{(K)} - U^{(K)}) = \sum_{i=1}^p S_i^K. \quad (37)$$

The values of S_i^K for the stage 1 calculation are also shown in Table 6. Subdomain 4 contributes the most towards the discretization error, and hence it is the prime

Table 6 Two stage solution strategy using multiplicative Schwarz to solve Poisson's equation: $\beta = 0.2$, $K = 6$

Stage	Num. vertices	Est. Err.	γ	$e_D^{\{K\}}$	γ_D	$e_I^{\{K\}}$
1	121	2.36e-03	9.83e-01	2.36e-03	9.89e-01	6.98e-06
2	253	3.44e-04	1.00e+00	3.37e-04	1.05e+00	6.97e-06
Stage	Num. vertices	i	1	2	3	4
1	121	S_i^K	3.07e-04	-7.94e-04	-7.82e-04	3.62e-03
2	253	S_i^K	1.82e-04	-3.87e-04	-3.85e-04	9.27e-04

**Fig. 3** **a** Initial uniform mesh. **b** Mesh refinement in Ω_4 guided by adjoint based error estimates. **c** Uniformly refined mesh

candidate for refinement. After refining all the elements in subdomain 4, the refined mesh is shown in Fig. 3b. The discretization errors in each subdomain S_i^K and the total error after the refinement are shown in Table 6. The discretization error is significantly lower and hence the total error is also significantly lower. The values of S_i^K also indicate that now each subdomain contributes roughly the same magnitude towards the discretization error.

We note that we can take advantage of cancellation of the discretization errors. Applying the standard approximation theory for degree one Lagrange finite elements, we expect the discretization error component S_4^K to decrease by a factor of four if we refine the mesh corresponding to subdomain 4 uniformly. The conjectured value for S_4^K is therefore approximately 9×10^{-4} . The discretization errors from subdomains 2 and 3 (represented by S_2^K and S_3^K) have negative signs and are not expected to change as significantly when subdomain 4 is refined. As shown in Table 6, after refinement of subdomain 4, there is significant cancellation of error between subdomains 2 and 3 and subdomain 4, and the total error is 3.44×10^{-4} . Uniformly refining the entire initial mesh results in a refined mesh with 441 vertices (shown in Fig. 3c) and the solution after $K = 6$ iterations has a total error of 6.24×10^{-4} , which is approximately the expected four-fold reduction in error. The mesh refined using adjoint based error information in Fig. 3b has almost half the number of degree of freedoms of the uniformly refined mesh in Fig. 3c, but none-the-less has half the total error (3.44×10^{-4} vs. 6.24×10^{-4}). Recognizing and taking advantage of cancellation of error can produce otherwise startling efficiencies. Similar refinement strategies, where specific “compo-

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

Stage	N_x	N_y	β	K	Est. Err.	γ	$e_D^{(K)}$	γ_D	$e_I^{(K)}$
1	40	40	0.05	2	1.23e-03	1.00e+00	1.79e-04	9.99e-01	1.05e-03
2	40	40	0.2	2	5.04e-04	1.00e+00	1.62e-04	9.99e-01	3.42e-04

nents" are refined to exploit cancellation of error, are also employed in [10,11]. Such component-wise refinement strategies allow for estimation of the decrease of error in a more reliable manner than classical adaptive refinement strategies in which disparate elements are marked for refinement.

4.5.2 Dominant iteration error

For the same choice of QoI, we perform a stage 1 computation with 2×2 subdomains and $N_x = N_y = 40$, $\beta = 0.05$ and $K = 2$. This configuration is shown in Fig. 2b. 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 β . We choose the latter option and set $\beta = 0.2$, see Fig. 2c. The results are shown in Table 7, where now the iteration error and discretization are balanced and the overall error has decreased.

5 Numerical examples for additive Schwarz

We repeat analogous numerical examples in Sect. 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 $\Phi_i^{[k]}$ in the expressions in Sect. 4.1, where $\Phi_i^{[k]}$ is the numerical approximation to $\phi_i^{[k]}$. A relaxation parameter $\tau = 0.4$ was used in all examples. The error estimates are again highly accurate with effectivity ratios close to 1.

5.1 Estimates for Poisson's equation

5.1.1 2×1 subdomains

We solve the same problem described in Sect. 4.2.1 by equations (31) and (32) using additive Schwarz. The results are shown in Table 8. In comparison to the results in Sect. 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 8 Additive Schwarz for Poisson's equation: 2×1 subdomains

N_x	N_y	β	K	Est. Err.	γ	$e_D^{(K)}$	γ_D	$e_I^{(K)}$
20	20	0.1	2	1.09e-02	1.00e+00	4.52e-04	9.98e-01	1.05e-02
20	20	0.2	2	1.04e-02	1.00e+00	4.34e-04	9.98e-01	9.96e-03
20	20	0.1	2	1.09e-02	1.00e+00	4.52e-04	9.98e-01	1.05e-02
20	20	0.1	4	4.23e-03	9.99e-01	6.02e-04	9.98e-01	3.62e-03
20	20	0.1	6	1.93e-03	9.99e-01	6.46e-04	9.98e-01	1.28e-03
20	20	0.1	2	1.09e-02	1.00e+00	4.52e-04	9.98e-01	1.05e-02
40	40	0.1	2	1.06e-02	1.00e+00	1.14e-04	9.99e-01	1.05e-02
80	80	0.1	2	1.05e-02	1.00e+00	2.85e-05	1.00e+00	1.05e-02

Table 9 Additive Schwarz for Poisson's equation: 4×1 subdomains

N_x	N_y	β	K	Est. Err.	γ	$e_D^{(K)}$	γ_D	$e_I^{(K)}$
20	20	0.1	2	1.89e-02	1.00e+00	5.42e-04	9.96e-01	1.84e-02
20	20	0.2	2	1.19e-02	1.00e+00	6.04e-04	9.97e-01	1.13e-02
20	20	0.1	2	1.89e-02	1.00e+00	5.42e-04	9.96e-01	1.84e-02
20	20	0.1	4	1.21e-02	1.00e+00	6.51e-04	9.97e-01	1.14e-02
20	20	0.1	6	7.90e-03	1.00e+00	6.84e-04	9.97e-01	7.22e-03
20	20	0.1	2	1.89e-02	1.00e+00	5.42e-04	9.96e-01	1.84e-02
40	40	0.1	2	1.85e-02	1.00e+00	1.38e-04	9.99e-01	1.84e-02
80	80	0.1	2	1.84e-02	1.00e+00	3.46e-05	1.00e+00	1.84e-02

5.1.2 4×1 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.

5.1.3 4×4 subdomains

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

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 Sect. 4.4 by equations (34) and (35). We provide results for two different configurations of the subdomains in Table 11 below.

Table 10 Additive Schwarz for Poisson's equation: 4×4 subdomains

N_x	N_y	β	K	Est. Err.	γ	$e_D^{\{K\}}$	γ_D	$e_I^{\{K\}}$
20	20	0.1	2	2.18e-02	1.00e+00	6.83e-04	1.00e+00	2.12e-02
20	20	0.2	2	1.25e-02	1.00e+00	6.14e-04	1.00e+00	1.18e-02
20	20	0.1	2	2.18e-02	1.00e+00	6.83e-04	1.00e+00	2.12e-02
20	20	0.1	4	1.58e-02	1.00e+00	9.42e-04	9.86e-01	1.48e-02
20	20	0.1	6	1.15e-02	1.00e+00	1.04e-03	9.80e-01	1.05e-02
20	20	0.1	2	2.18e-02	1.00e+00	6.83e-04	1.00e+00	2.12e-02
40	40	0.1	2	2.13e-02	1.00e+00	1.70e-04	1.00e+00	2.12e-02
80	80	0.1	2	2.12e-02	1.00e+00	4.22e-05	1.00e+00	2.12e-02

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

K	Est. Err.	γ	$e_D^{\{K\}}$	γ_D	$e_I^{\{K\}}$
4×1 configuration					
2	1.78e-02	1.00e+00	-1.04e-04	9.92e-01	1.79e-02
4	1.28e-02	1.00e+00	-9.38e-05	9.81e-01	1.29e-02
6	8.40e-03	1.00e+00	-5.56e-05	9.54e-01	8.46e-03
1×4 configuration					
2	1.08e-02	1.00e+00	-1.32e-04	9.91e-01	1.10e-02
4	5.11e-03	1.00e+00	-2.37e-04	9.93e-01	5.35e-03
6	2.32e-03	1.00e+00	-3.01e-04	9.94e-01	2.62e-03

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 Dominant discretization error

We repeat the problem in Sect. 4.5.1 and the results are shown in Table 12. We observe the expected reduction in discretization error in subdomain 4, but the reduction in total error is not as dramatic as in the multiplicative Schwarz case. There is less cancellation between discretization errors of opposite sign following local mesh refinement, and the iteration error is much larger for additive Schwarz. However, after mesh refinement in subdomain 4 and six iterations, the iteration error makes the largest contribution to the total error.

Table 12 Two stage solution strategy using additive Schwarz to solve Poisson's equation: $\beta = 0.2$, $K = 6$

Stage	Num. vertices	Est. Err.	γ	$e_D^{\{K\}}$	γ_D	$e_I^{\{K\}}$
1	121	3.24e-03	9.88e-01	2.48e-03	9.90e-01	7.61e-04
2	253	1.24e-03	1.00e+00	4.79e-04	1.04e+00	7.60e-04
Stage	Num. vertices	i	1	2	3	4
1	121	S_i^K	6.82e-05	-3.76e-04	-3.76e-04	3.16e-03
2	253	S_i^K	4.13e-05	-1.78e-04	-1.78e-04	7.93e-04

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

N_x	N_y	β	K	Est. Err.	γ	$e_D^{\{K\}}$	γ_D	$e_I^{\{K\}}$
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

5.3.2 Dominant iteration error

The results upon repeating the problem in Sect. 4.5.2 are shown in Table 13. Increasing the overlap reduces the iteration error, but not as effectively as for multiplicative Schwarz, and after only two iterations the iteration error remains significantly larger than the discretization error.

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

6.1 Analogy with algebraic Gauss-Seidel iteration

It is helpful to consider an algebraic analog of multiplicative Schwarz overlapping domain decomposition in order to provide insight in to the unusual forms of equations (22) and (23) and Theorem 3. Consider solving the algebraic linear system $Mx = b$, where M is a $p \times p$ matrix, using K Gauss-Seidel iterations. (Here we choose $p = 4$ and $K = 5$.)

We decompose the matrix M as a sum of strictly lower triangular, diagonal and a strictly upper triangular matrices as $M = L + D + U$ and solve

$$(L + D)x^{[k+1]} = b - Ux^{[k]}, k = 0, 1, \dots$$

Let $A = (L + D)$ and $B = U$, each of which are $p \times p$ matrices. The complete Gauss-Seidel iteration can be written as the following block lower triangular system

$$C_{\text{gs}}x = b,$$

$$C_{\text{gs}} = \begin{bmatrix} A & 0 & 0 & 0 & 0 \\ B & A & 0 & 0 & 0 \\ 0 & B & A & 0 & 0 \\ 0 & 0 & B & A & 0 \\ 0 & 0 & 0 & B & A \end{bmatrix}.$$
$$\mathbf{x}^\top = (x^{\{1\}\top}, x^{\{2\}\top}, x^{\{3\}\top}, x^{\{4\}\top}, x^{\{5\}\top}) \quad \text{and} \quad \mathbf{b}^\top = (b^\top, b^\top, b^\top, b^\top, b^\top).$$
$$C_{\text{gs}}^{\top} = \begin{bmatrix} A^{\top} & B^{\top} & 0 & 0 & 0 \\ 0 & A^{\top} & B^{\top} & 0 & 0 \\ 0 & 0 & A^{\top} & B^{\top} & 0 \\ 0 & 0 & 0 & A^{\top} & B^{\top} \\ 0 & 0 & 0 & 0 & A^{\top} \end{bmatrix}.$$
$$\phi^\top = (\phi_1, \phi_2, \phi_3, \phi_4, \phi_5)^\top.$$
$$A^\top \phi_5 = \psi, \\ A^\top \phi_4 = -B^\top \phi_5, \quad A^\top \phi_3 = -B^\top \phi_4, \quad A^\top \phi_2 = -B^\top \phi_3, \quad A^\top \phi_1 = -B^\top \phi_2,$$
$$C_{\text{gs}} = \begin{bmatrix} A_{11} & & & & & & & & \\ A_{21} & A_{22} & & & & & & & \\ A_{31} & A_{32} & A_{33} & & & & & & \\ A_{41} & A_{42} & A_{43} & A_{44} & & & & & \\ - & A_{12} & A_{13} & A_{14} & A_{11} & & & & \\ & A_{23} & A_{24} & A_{21} & A_{22} & & & & \\ & & A_{34} & A_{31} & A_{32} & A_{33} & & & \\ - & & & A_{41} & A_{42} & A_{43} & A_{44} & & \\ & & & & & & \vdots & \dots & \end{bmatrix},$$

$$C_{gs}^T = \begin{bmatrix} A_{11}^T & A_{21}^T & A_{31}^T & A_{41}^T & & & \\ & A_{22}^T & A_{32}^T & A_{42}^T & & & \\ & & A_{33}^T & A_{43}^T & & & \\ & & & A_{44}^T & & & \\ & & & & A_{11}^T & A_{21}^T & A_{31}^T & A_{41}^T \\ & & & & & A_{22}^T & A_{32}^T & A_{42}^T \\ & & & & & & A_{33}^T & A_{43}^T \\ & & & & & & & A_{44}^T \\ & & & & & & & & \ddots & \dots \end{bmatrix},$$

and the adjoint equations within each block can also be solved via backward substitution. The adjoint equations are therefore

$$A_{ii}^T \phi_i^{[K]} = \psi_i - \sum_{j>i} A_{ji}^T \phi_j^{[K]}, \quad i = 1, \dots, p, \quad (38)$$

$$A_{ii}^T \phi_i^{[k]} = - \sum_{j<i} A_{ji}^T \phi_j^{[k+1]} - \sum_{j>i} A_{ji}^T \phi_j^{[k]}, \quad i = 1, \dots, p, \quad k = K-1, \dots, 1. \quad (39)$$

The form of the adjoint problems in (38) and (39) mimic those in equations (22) and (23). The sum on the RHS of (38) represents the additional adjoint problems that must be solved to estimate effect of errors made while solving forward problems during the final (K th) iteration. We call these *within iteration* transfer errors. The first sum on the RHS of (39) represents the additional adjoint problems that must be solved to estimate the effect of errors made while solving forward problems during the previous iteration. We call these *between iteration* transfer errors. The second sum on the RHS of (39) again represents additional adjoint problems to estimate *within iteration* transfer errors. These two distinct types of transfer error were earlier identified in the context of operator decomposition approaches to coupled semilinear elliptic systems in [7]. Since $C_{gs}x = b$ is just a $Kp \times Kp$ linear system,

$$(e, \psi) = (\mathcal{R}, \phi) \quad (40)$$

where

$$\mathcal{R} = b - C_{gs}\hat{x}$$

for approximate solution \hat{x} . The error in the quantity of interest can be expressed as an inner products of two vectors of length Kp , and (40) mimics the result in equation (24).

6.2 Details of analysis of multiplicative Schwarz algorithm

6.2.1 Reformulation of the algorithm

Algorithm 1 is not amenable to adjoint based analysis since the affine solution space $H_{D_k}^1(\Omega_i)$ changes at every iteration. We reformulate the algorithm by using a standard lifting technique to account for this in Algorithm 5. We set

$$\tilde{u}^{\{k+i/p\}} = w^{\{k+i/p\}} + u^{\{k+(i-1)/p\}} \quad \text{on } \Omega_i, \quad (41)$$

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

Algorithm 5 Reformulated overlapping multiplicative Schwarz

Given $u^{(0)}$ defined on Ω
for $k = 0, 1, 2, \dots, K-1$ **do**
 for $i = 1, 2, \dots, p$ **do**
 Find $w^{\{k+i/p\}} \in H_0^1(\Omega_i)$ such that

$$a_i(w^{\{k+i/p\}}, v) = l_i(v) - a_i(u^{\{k+(i-1)/p\}}, v), \quad \forall v \in H_0^1(\Omega_i). \quad (42)$$

Let

$$u^{\{k+i/p\}} = \begin{cases} u^{\{k+(i-1)/p\}} + w^{\{k+i/p\}}, & \text{on } \overline{\Omega}_i, \\ u^{\{k+(i-1)/p\}}, & \text{on } \Omega \setminus \overline{\Omega}_i. \end{cases} \quad (43)$$

end for
end for

There is an equivalent reformulation of the discrete Algorithm 5 and we denote the unknown solutions as $W^{\{k+i/p\}}$ belonging to the spaces $V_{i,h,0} \subset H_0^1(\Omega_i)$. The solutions $W^{\{k+i/p\}}$ are defined formally for the analysis but are not computed in practice.

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

6.2.2 Technical lemmas

Let $e_W^{\{k\}} = w^{\{k\}} - W^{\{k\}}$. By (41) we have

$$e_W^{\{k+i/p\}} = e_D^{\{k+i/p\}} - e_D^{\{k+(i-1)/p\}} \quad \text{on } \Omega_i. \quad (44)$$

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

Lemma 2 (Error in QoI in terms of discretization errors with homogeneous bcs)

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

Notation	Formula	Space	Meaning
u		$H_0^1(\Omega)$	True solution
$u^{[k]}$		$H_0^1(\Omega_i)$	Global analytic solution at iteration k
$U^{[k]}$		V_h	Global discrete solution at iteration k
$\tilde{u}^{\{k+i/p\}}$		$H_{D_k}^1(\Omega_i)$	Analytic solutions on Ω_i at iteration k
$\tilde{U}^{\{k+i/p\}}$		$V_{i,h}^k$	Discrete solutions on Ω_i at iteration k
$w^{\{k+i/p\}}$		$H_0^1(\Omega_i)$	Analytic solns on Ω_i with homogen. bcs at iteration k
$W^{\{k+i/p\}}$		$V_{i,h,0}$	Discrete solns on Ω_i with homogen. bcs at iteration k
$e^{[k]}$	$u - U^{[k]}$	$H_0^1(\Omega)$	Total error
$e_I^{[k]}$	$u - u^{[k]}$	$H_0^1(\Omega)$	Global iteration error at iteration k
$e_D^{[k]}$	$u^{[k]} - U^{[k]}$	$H_0^1(\Omega)$	Global discretization error at iteration k
$e_W^{\{k+i/p\}}$	$w^{\{k+i/p\}} - W^{\{k+i/p\}}$	$H_0^1(\Omega_i)$	Discretization error on Ω_i with homogen. bcs at it. k

The discretization error in the QoI is

$$\left(e_D^{\{K\}}, \psi\right) = \sum_{k=0}^{K-1} \sum_{i=1}^p \sum_{j=1}^p \left(e_W^{\{k+i/p\}}, \psi_j\right)_{ij}. \quad (45)$$

Proof From equation (44) and the fact that $\psi_j = 0$ on $\Omega \setminus \Omega_j$ for fixed j we have

$$\begin{aligned} \left(e_D^{\{K\}}, \psi_j\right) &= \left(e_D^{\{K-1+p/p\}}, \psi_j\right) \\ &= \left(e_W^{\{K-i+p/p\}}, \psi_j\right)_{pj} + \left(e_D^{\{K-1+(p-1)/p\}}, \psi_j\right) \\ &= \left(e_W^{\{K-i+p/p\}}, \psi_j\right)_{pj} + \left(e_W^{\{K-i+(p-1)/p\}}, \psi_j\right)_{(p-1)j} \\ &\quad + \left(e_D^{\{K-1+(p-2)/p\}}, \psi_j\right). \end{aligned}$$

Continuing,

$$\left(e_D^{\{K\}}, \psi_j\right) = \left(e_D^{\{K-1\}}, \psi_j\right) + \sum_{i=1}^p \left(e_W^{\{K-1+i/p\}}, \psi_j\right)_{ij}.$$

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

$$\left(e_D^{\{K\}}, \psi_j\right) = \sum_{k=0}^{K-1} \sum_{i=1}^p \left(e_W^{\{k+i/p\}}, \psi_j\right)_{ij}.$$

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

$$\sum_{j=1}^p \left(e_D^{\{K\}}, \psi_j \right) = \sum_{k=0}^{K-1} \sum_{i=1}^p \sum_{j=1}^p \left(e_W^{\{k+i/p\}}, \psi_j \right)_{ij}.$$

□

Lemma 3 (Bilinear form with discretization errors with homogeneous bcs) *For any $v \in H_{D_k}^1(\Omega_i)$ we have*

$$a_i \left(e_W^{\{i/p\}}, v \right) = a_i \left(e_D^{\{i/p\}}, v \right) - \sum_{r=1}^{i-1} a_{ir} \left(e_W^{\{r/p\}}, v \right). \quad (46)$$

and for $k \geq 1$,

$$\begin{aligned} a_i \left(e_W^{\{k+i/p\}}, v \right) &= a_i \left(e_D^{\{k+i/p\}}, v \right) - a_i \left(e_D^{\{k-1+i/p\}}, v \right) - \sum_{r=1}^{i-1} a_{ir} \left(e_W^{\{k+r/p\}}, v \right) \\ &\quad - \sum_{r=i+1}^p a_{ir} \left(e_W^{\{k-1+r/p\}}, v \right). \end{aligned} \quad (47)$$

Proof By (44) we have for $m < i$,

$$\begin{aligned} a_i \left(e_D^{\{m/p\}}, v \right) &= a_i \left(e_D^{\{(m-1)/p\}}, v \right) + a_{i,m} \left(e_W^{\{m/p\}}, v \right), \\ &= a_i \left(e_D^{\{(m-2)/p\}}, v \right) + a_{i,m-1} \left(e_W^{\{(m-1)/p\}}, v \right) + a_{i,m} \left(e_W^{\{m/p\}}, v \right). \end{aligned}$$

where we use $e_W^{\{r/p\}} = 0$ on $\Omega \setminus \Omega_r$. Continuing in this manner yields

$$a_i \left(e_D^{\{m/p\}}, v \right) = a_i \left(e_D^{\{0\}}, v \right) + \sum_{r=1}^m a_{ir} \left(e_W^{\{r/p\}}, v \right) = \sum_{r=1}^m a_{ir} \left(e_W^{\{r/p\}}, v \right), \quad (48)$$

since $e_D^{\{0\}} = 0$. Again by (44),

$$a_i \left(e_W^{\{i/p\}}, v \right) = a_i \left(e_D^{\{i/p\}}, v \right) - a_i \left(e_D^{\{(i-1)/p\}}, v \right). \quad (49)$$

Using (48) with $m = i - 1$ with (49) leads to

$$a_i \left(e_W^{\{i/p\}}, v \right) = a_i \left(e_D^{\{i/p\}}, v \right) - \sum_{r=1}^{i-1} a_{ir} \left(e_W^{\{r/p\}}, v \right),$$

thus showing (46). A similar argument shows (47) for $k \geq 1$.

□

Lemma 4 (Sums of bilinear form with discretization errors with homogeneous bcs)
 For $0 \leq Q \leq K - 1$ we have

$$\begin{aligned} \sum_{k=0}^Q a_i \left(e_W^{\{k+i/p\}}, v \right) &= a_i \left(e_D^{\{Q+i/p\}}, v \right) \\ &\quad - \sum_{k=0}^Q \sum_{r=1}^{i-1} a_{ir} \left(e_W^{\{k+r/p\}}, v \right) - \sum_{k=0}^{Q-1} \sum_{r=i+1}^p a_{ir} \left(e_W^{\{k+r/p\}}, v \right). \end{aligned} \quad (50)$$

Proof By Lemma 3,

$$\begin{aligned} \sum_{k=0}^Q a_i \left(e_W^{\{k+i/p\}}, v \right) &= \sum_{k=1}^Q a_i \left(e_W^{\{k+i/p\}}, v \right) + a_i \left(e_W^{\{i/p\}}, v \right) \\ &= \sum_{k=1}^Q \left\{ a_i \left(e_D^{\{k+i/p\}}, v \right) - a_i \left(e_D^{\{k-1+i/p\}}, v \right) \right. \\ &\quad \left. - \sum_{r=1}^{i-1} a_{ir} \left(e_W^{\{k+r/p\}}, v \right) - \sum_{r=i+1}^p a_{ir} \left(e_W^{\{k-1+r/p\}}, v \right) \right\} \\ &\quad + a_i \left(e_D^{\{i/p\}}, v \right) - \sum_{r=1}^{i-1} a_{ir} \left(e_W^{\{r/p\}}, v \right) \\ &= \sum_{k=1}^Q \left\{ a_i \left(e_D^{\{k+i/p\}}, v \right) - a_i \left(e_D^{\{k-1+i/p\}}, v \right) \right\} + a_i \left(e_D^{\{i/p\}}, v \right) \\ &\quad - \sum_{k=1}^Q \sum_{r=1}^{i-1} a_{ir} \left(e_W^{\{k+r/p\}}, v \right) - \sum_{r=1}^{i-1} a_{ir} \left(e_W^{\{r/p\}}, v \right) - \sum_{k=1}^Q \sum_{r=i+1}^p a_{ir} \left(e_W^{\{k-1+r/p\}}, v \right) \\ &= a_i \left(e_D^{\{Q+i/p\}}, v \right) - \sum_{k=0}^Q \sum_{r=1}^{i-1} a_{ir} \left(e_W^{\{k+r/p\}}, v \right) \\ &\quad - \sum_{k=0}^{Q-1} \sum_{r=i+1}^p a_{ir} \left(e_W^{\{k+r/p\}}, v \right). \end{aligned}$$

□

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*

$$\begin{aligned} & \sum_{k=0}^Q \tau_R^Q \left(e_W^{\{k+R/p\}} \right) - \sum_{k=0}^Q \sum_{j=M}^p a_{Rj} \left(e_W^{\{k+R/p\}}, \phi^{\{Q+j/p\}} \right) \\ &= a_R \left(e_D^{\{Q+R/p\}}, \phi^{\{Q+R/p\}} \right) - \sum_{k=0}^Q \sum_{i=1}^{R-1} a_{iR} \left(e_W^{\{k+i/p\}}, \phi^{\{Q+R/p\}} \right) \\ & \quad - \sum_{k=0}^{Q-1} \sum_{i=M}^p a_{iR} \left(e_W^{\{k+i/p\}}, \phi^{\{Q+R/p\}} \right). \end{aligned}$$

Proof From the adjoint equation (22) we have

$$a_R \left(e_W^{\{k+R/p\}}, \phi^{\{Q+R/p\}} \right) = \tau_i^Q \left(e_W^{\{k+R/p\}} \right) - \sum_{j=M}^p a_{Ri} \left(e_W^{\{k+R/p\}}, \phi^{\{Q+j/p\}} \right). \quad (51)$$

From Lemma 4,

$$\begin{aligned} & \sum_{k=0}^Q a_R \left(e_W^{\{k+R/p\}}, \phi^{\{Q+R/p\}} \right) \\ &= a_R \left(e_D^{\{Q+R/p\}}, \phi^{\{Q+R/p\}} \right) - \sum_{k=0}^Q \sum_{i=1}^{R-1} a_{iR} \left(e_W^{\{k+i/p\}}, \phi^{\{Q+R/p\}} \right) \\ & \quad - \sum_{k=0}^{Q-1} \sum_{i=M}^p a_{iR} \left(e_W^{\{k+i/p\}}, \phi^{\{Q+R/p\}} \right). \end{aligned} \quad (52)$$

Combining (51) and (52) proves the result. \square

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,*

$$\begin{aligned} I &= \sum_{k=0}^Q \sum_{i=1}^p \tau_i^Q \left(e_W^{\{k+i/p\}} \right) = \sum_{i=M}^p a_i \left(e_D^{\{Q+i/p\}}, \phi^{\{Q+i/p\}} \right) + \sum_{k=0}^Q \sum_{i=1}^{M-1} \tau_i^Q \left(e_W^{\{k+i/p\}} \right) \\ & \quad - \sum_{k=0}^Q \sum_{i=1}^{M-1} \sum_{j=M}^p a_{ij} \left(e_W^{\{k+i/p\}}, \phi^{\{Q+j/p\}} \right) \\ & \quad - \sum_{k=0}^{Q-1} \sum_{i=M+1}^p \sum_{j=M}^{i-1} a_{ij} \left(e_W^{\{k+i/p\}}, \phi^{\{Q+j/p\}} \right). \end{aligned} \quad (53)$$

Proof The proof is by induction on M .

[I] For $M = p + 1$ the right-hand side of (53) 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 $e_W^{\{k+(M-1)/p\}}$.

$$\begin{aligned}
 I &= \sum_{i=M}^p a_i \left(e_D^{\{Q+i/p\}}, \phi^{\lfloor Q+i/p \rfloor} \right) + \sum_{k=0}^Q \sum_{i=1}^{M-2} \tau_i^Q \left(e_W^{\{k+i/p\}} \right) \\
 &\quad - \sum_{k=0}^Q \sum_{i=1}^{M-2} \sum_{j=M}^p a_{i,j} \left(e_W^{\{k+i/p\}}, \phi^{\lfloor Q+j/p \rfloor} \right) \\
 &\quad - \sum_{k=0}^{Q-1} \sum_{i=M+1}^p \sum_{j=M}^{i-1} a_{i,j} \left(e_W^{\{k+i/p\}}, \phi^{\lfloor Q+j/p \rfloor} \right) + \sum_{k=0}^Q \tau_{M-1}^Q \left(e_W^{\{k+(M-1)/p\}} \right) \\
 &\quad - \sum_{k=0}^Q \sum_{j=M}^p a_{M-1,j} \left(e_W^{\{k+(M-1)/p\}}, \phi^{\lfloor Q+j/p \rfloor} \right). \tag{54}
 \end{aligned}$$

From Lemma 5,

$$\begin{aligned}
 &\sum_{k=0}^Q \tau_{M-1}^Q \left(e_W^{\{k+(M-1)/p\}} \right) - \sum_{k=0}^Q \sum_{j=M}^p a_{M-1,j} \left(e_W^{\{k+(M-1)/p\}}, \phi^{\lfloor Q+j/p \rfloor} \right) \\
 &= a_{M-1} \left(e_D^{\{Q+(M-1)/p\}}, \phi^{\lfloor Q+(M-1)/p \rfloor} \right) - \sum_{k=0}^Q \sum_{i=1}^{M-2} a_{i,M-1} \left(e_W^{\{k+i/p\}}, \phi^{\lfloor Q+(M-1)/p \rfloor} \right) \\
 &\quad - \sum_{k=0}^{Q-1} \sum_{i=M}^p a_{i,M-1} \left(e_W^{\{k+i/p\}}, \phi^{\lfloor Q+(M-1)/p \rfloor} \right). \tag{55}
 \end{aligned}$$

Combining (55) with (54),

$$\begin{aligned}
 I &= \sum_{i=M-1}^p a_i \left(e_D^{\{Q+i/p\}}, \phi^{\lfloor Q+i/p \rfloor} \right) + \sum_{k=0}^Q \sum_{i=1}^{M-2} \tau_i^Q \left(e_W^{\{k+i/p\}} \right) \\
 &\quad - \sum_{k=0}^Q \sum_{i=1}^{M-2} \sum_{j=M-1}^p a_{i,j} \left(e_W^{\{k+i/p\}}, \phi^{\lfloor Q+j/p \rfloor} \right) \\
 &\quad - \sum_{k=0}^{Q-1} \sum_{i=M}^p \sum_{j=M-1}^{i-1} a_{i,j} \left(e_W^{\{k+i/p\}}, \phi^{\lfloor Q+j/p \rfloor} \right).
 \end{aligned}$$

□

Corollary 1 Let $0 \leq Q < K$. Then we have

$$\sum_{k=0}^Q \sum_{i=1}^p \tau_i^Q \left(e_W^{\{k+i/p\}} \right) = \sum_{i=1}^p a_i \left(e_D^{\{Q+i/p\}}, \phi^{[Q+i/p]} \right) + \sum_{k=0}^{Q-1} \sum_{i=1}^p \tau_i^{Q-1} \left(e_W^{\{k+i/p\}} \right). \quad (56)$$

Proof Set $M = 1$ in Lemma 6 to get,

$$\begin{aligned} \sum_{k=0}^Q \sum_{i=1}^p \tau_i^Q \left(e_W^{\{k+i/p\}} \right) &= \sum_{i=1}^p a_i \left(e_D^{\{Q+i/p\}}, \phi^{[Q+i/p]} \right) \\ &\quad - \sum_{k=0}^{Q-1} \sum_{i=2}^p \sum_{j=1}^{i-1} a_{ij} \left(e_W^{\{k+i/p\}}, \phi^{[Q+j/p]} \right) \\ &= \sum_{i=1}^p a_i \left(e_D^{\{Q+i/p\}}, \phi^{[Q+i/p]} \right) - \sum_{k=0}^{Q-1} \sum_{i=2}^p \tau_i^{Q-1} \left(e_W^{\{k+i/p\}} \right) \\ &= \sum_{i=1}^p a_i \left(e_D^{\{Q+i/p\}}, \phi^{[Q+i/p]} \right) - \sum_{k=0}^{Q-1} \sum_{i=1}^p \tau_i^{Q-1} \left(e_W^{\{k+i/p\}} \right), \end{aligned} \quad (57)$$

where we use (23) and note that $\tau_1^Q(v) = 0$ for $Q < K - 1$. \square

6.2.3 Proof of Theorem 3

Proof From Lemma 2 and (23),

$$\left(e_D^{\{K\}}, \psi \right) = \sum_{k=0}^{K-1} \sum_{i=1}^p \sum_{j=1}^p \left(e_W^{\{k+i/p\}}, \psi_j \right)_{ij} = \sum_{k=0}^{K-1} \sum_{i=1}^p \tau_i^{K-1} \left(e_W^{\{k+i/p\}} \right).$$

Applying Corollary 1 yields

$$\left(e^{\{K\}}, \psi \right) = \sum_{i=1}^p a_i \left(e_D^{\{K-1+i/p\}}, \phi^{[K-1+i/p]} \right) - \sum_{k=0}^{K-2} \sum_{i=1}^p \tau_i^{K-2} \left(e_W^{\{k+i/p\}} \right).$$

Repeated application of Corollary 1 yields

$$\left(e^{\{K\}}, \psi \right) = \sum_{k=0}^{K-1} \sum_{i=1}^p a_i \left(e_D^{\{k+i/p\}}, \phi^{[k+i/p]} \right). \quad (58)$$

Now,

$$\begin{aligned}
 a_i \left(e_D^{\{k+i/p\}}, \phi^{\{k+i/p\}} \right) &= a_i \left(u^{\{k+i/p\}} - U^{\{k+i/p\}}, \phi^{\{k+i/p\}} \right) \\
 &= a_i \left(\tilde{u}^{\{k+i/p\}}, \phi^{\{k+i/p\}} \right) - a_i \left(\tilde{U}^{\{k+i/p\}}, \phi^{\{k+i/p\}} \right) \\
 &= l_i \left(\phi^{\{k+i/p\}} \right) - a_i \left(\tilde{U}^{\{k+i/p\}}, \phi^{\{k+i/p\}} \right) = R_i \left(\tilde{U}^{\{k+i/p\}}, \phi^{\{k+i/p\}} \right).
 \end{aligned} \tag{59}$$

Combining (58) and (59) leads to

$$\left(\psi, u^{\{K\}} - U^{\{K\}} \right) = \sum_{k=0}^{K-1} \sum_{i=1}^p R_i \left(\tilde{U}^{\{k+i/p\}}, \phi^{\{k+i/p\}} \right). \tag{60}$$

The discrete equivalent of (9) is

$$R_i \left(\tilde{U}^{\{k+i/p\}}, v \right) = l_i(v) - a_i \left(\tilde{U}^{\{k+i/p\}}, v \right), \quad \forall v \in V_{i,h,0}. \tag{61}$$

Substituting $v = \pi_i \phi^{\{k+i/p\}} \in V_{i,h,0}$ in (61) and subtracting the result from (60) completes the proof. \square

6.3 Details of analysis of additive Schwarz algorithm

6.3.1 Reformulation of the algorithm

Similar to the multiplicative case in Sect. 6.2, the basic additive algorithm 2 is not amenable to adjoint based analysis since the affine solution space $H_{D_k}^1(\Omega_i)$ changes at every iteration. We reformulate the algorithm by again using a standard lifting technique to account for this. We set

$$\tilde{u}_i^{\{k+1\}} = w_i^{\{k+1\}} + u^{\{k\}} \quad \text{on } \Omega_i, \tag{62}$$

where now $w_i^{\{k+1\}} \in H_0^1(\Omega_i)$. This results in Algorithm 6.

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

Notation	Formula	Space	Meaning
u		$H_0^1(\Omega)$	True solution
$u^{[k]}$		$H_0^1(\Omega_i)$	Global analytic solution at iteration k
$U^{[k]}$		V_h	Global discrete solution at iteration k
$\tilde{u}_i^{[k]}$		$H_{D_k}^1(\Omega_i)$	Analytic solutions on Ω_i at iteration k
$\tilde{U}_i^{[k]}$		$V_{i,h}^k$	Discrete solutions on Ω_i at iteration k
$w_i^{[k]}$		$H_0^1(\Omega_i)$	Analytic solns on Ω_i with homogen. bcs at iteration k
$W^{[k]}$		$V_{i,h,0}$	Discrete solns on Ω_i with homogen. bcs at iteration k
$e^{[k]}$	$u - U^{[k]}$	$H_0^1(\Omega)$	Total error
$e_I^{[k]}$	$u - u^{[k]}$	$H_0^1(\Omega)$	Global iteration error at iteration k
$e_D^{[k]}$	$u^{[k]} - U^{[k]}$	$H_0^1(\Omega)$	Global discretization error at iteration k
$e_{W,i}^{[k]}$	$w_i^{[k]} - W_i^{[k]}$	$H_0^1(\Omega_i)$	Discretization error on Ω_i with homogen. bcs at it. k

Algorithm 6 Reformulated overlapping additive Schwarz

Given $u^{[0]}$ defined on Ω
for $k = 0, 1, 2, \dots, K - 1$ **do**
 for $i = 1, 2, \dots, p$ **do**
 Find $w_i^{[k+1]} \in H_0^1(\Omega_i)$ such that

$$a_i(w_i^{[k+1]}, v) = l_i(v) - a_i(u^{[k]}, v), \quad \forall v \in H_0^1(\Omega_i). \quad (63)$$

Let

$$u^{[k+1]} = u^{[k]} + \tau \left(\sum_{i=1}^p \tilde{\Pi}_i w_i^{[k+1]} \right) \text{ where } \tilde{\Pi}_i w_i^{[k+1]} = \begin{cases} w_i^{[k+1]}, & \text{on } \overline{\Omega}_i, \\ 0, & \text{on } \Omega \setminus \overline{\Omega}_i. \end{cases} \quad (64)$$

end for
end for

There is an equivalent reformulation of the discrete Algorithm 6 and we denote the unknown solutions as $W^{[k]}$ belonging to the spaces $V_{i,h,0} \subset H_0^1(\Omega_i)$. These solutions are defined formally but are not computed in practice. Equation (64), which shows that $u^{[k+1]}$ is a weighted sum of all previous solutions to (63), results in very different adjoint problems for additive Schwarz (equations (25)) from those for multiplicative Schwarz (equations (22) and (23)).

To distinguish between different solutions (true, analytical, discrete) we use the notation in Table 15.

6.3.2 Technical lemmas

Let $e_W^{\{k\}} = w^{\{k\}} - W^{\{k\}}$. By (64) we have

$$e_D^{\{k\}} = e_D^{\{k-1\}} + \tau \sum_{i=1}^p \tilde{\Pi}_i e_{W,i}^{\{k\}}. \quad (65)$$

We apply lemma 1 to arrive at

$$\left(e_D^{\{k\}}, \psi \right) = \left(e_D^{\{k\}}, \sum_{i=1}^p \chi_i \psi \right) = \sum_{i=1}^p \left(e_D^{\{k\}}, \psi_i \right)_{ii}. \quad (66)$$

Lemma 7 (Error in QoI in terms of discretization errors with homogeneous bcs)
The discretization error in the QoI is

$$\left(e_D^K, \psi \right) = \tau \sum_{k=1}^K \sum_{i=1}^p \sum_{j=1}^p \left(e_{W,i}^{\{k\}}, \psi_j \right)_{ij}.$$

Proof Using (65), we have for a fixed j

$$\left(e_D^{\{K\}}, \psi_j \right)_{jj} = \left(e_D^{\{K-1\}}, \psi_j \right)_{jj} + \tau \sum_{i=1}^p \left(e_{W,i}^{\{K\}}, \psi_j \right)_{ij},$$

This is a recursive relation involving $\hat{e}^{\{K\}}$. Unrolling the recursion leads to

$$\left(e_D^{\{K\}}, \psi_j \right)_{jj} = \tau \sum_{k=1}^K \sum_{i=1}^p \left(e_{W,i}^{\{k\}}, \psi_j \right)_{ij}.$$

Summing over all $j = 1, \dots, p$ and using (66),

$$\left(\hat{e}^{\{K\}}, \psi \right) = \tau \sum_{k=1}^K \sum_{i=1}^p \sum_{j=1}^p \left(e_{W,i}^{\{k\}}, \psi_j \right)_{ij}.$$

□

Lemma 8 [Bilinear form with global discretization errors] For any $v \in V_i$ we have

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

Proof By (65), we have

$$\begin{aligned} a_i \left(e_D^{\{k\}}, v \right) &= a_i \left(e_D^{\{k-1\}}, v \right) + \tau \sum_{j=1}^p a_{ij} \left(e_{W,j}^{\{k\}}, v \right) \\ &= a_i \left(e_D^{\{k-1\}}, v \right) + \tau \sum_{j=1}^p a_{ij} \left(e_{W,j}^{\{k\}}, v \right), \end{aligned}$$

since e_W is the identity on subdomain j . This is a recursive relation involving $a_i \left(e_D^{\{k\}}, v \right)$. Unrolling this recursion and using the fact that $e_D^{\{0\}} = 0$ proves the result. \square

Lemma 9 (Bilinear form with local discretization errors with homogeneous bcs)

$$a_i \left(e_{W,i}^{\{k\}}, \phi_i^{\{k\}} \right) = R_i \left(\tilde{U}_i^{\{k\}}, \phi_i^{\{k\}} \right) - \tau \sum_{m=1}^{k-1} \sum_{j=1}^p a_{ij} \left(e_{W,j}^{\{m\}}, \phi_i^{\{k\}} \right).$$

Proof By definition of $e_{W,i}^{\{k\}}$,

$$\begin{aligned} a_i \left(e_{W,i}^{\{k\}}, \phi_i^{\{k\}} \right) &= a_i \left(w_i^{\{k\}}, \phi_i^{\{k\}} \right) - a_i \left(W_i^{\{k\}}, \phi_i^{\{k\}} \right) \\ &= a_i \left(w_i^{\{k\}} + u_i^{\{k-1\}}, \phi_i^{\{k\}} \right) \\ &\quad - a_i \left(u_i^{\{k-1\}}, \phi_i^{\{k\}} \right) - a_i \left(W_i^{\{k\}} + U_i^{\{k-1\}}, \phi_i^{\{k\}} \right) + a_i \left(U_i^{\{k-1\}}, \phi_i^{\{k\}} \right). \end{aligned}$$

Using (62) followed by (63) and definition of $e_D^{\{k\}}$,

$$\begin{aligned} a_i \left(e_{W,i}^{\{k\}}, \phi_i^{\{k\}} \right) &= a_i \left(\tilde{u}_i^{\{k\}}, \phi_i^{\{k\}} \right) - a_i \left(u_i^{\{k-1\}}, \phi_i^{\{k\}} \right) - a_i \left(\tilde{U}_i^{\{k\}}, \phi_i^{\{k\}} \right) + a_i \left(U_i^{\{k-1\}}, \phi_i^{\{k\}} \right) \\ &= R_i \left(\tilde{U}_i^{\{k\}}, \phi_i^{\{k\}} \right) - a_i \left(e_D^{\{k-1\}}, \phi_i^{\{k\}} \right). \end{aligned}$$

By Lemma 8,

$$a_i \left(e_{W,i}^{\{k\}}, \phi_i^{\{k\}} \right) = R_i \left(\tilde{U}_i^{\{k\}}, \phi_i^{\{k\}} \right) - \tau \sum_{m=1}^{k-1} \sum_{j=1}^p a_{ij} \left(e_{W,j}^{\{m\}}, \phi_i^{\{k\}} \right).$$

\square

6.3.3 Proof of Theorem 4

Proof By (25),

$$\left(\psi, e_D^{\{K\}} \right) = \tau \sum_{k=1}^K \sum_{i=1}^p \sum_{j=1}^p \left(\psi_j, e_{W,i}^{\{k\}} \right)_{ij}$$

$$= \sum_{k=1}^K \sum_{i=1}^p \left\{ a_i \left(e_{W,i}^{\{k\}}, \phi_i^{\{k\}} \right) + \tau \sum_{j=1}^p \sum_{l=k+1}^K a_{ij} \left(e_{W,i}^{\{k\}}, \phi_j^{\{l\}} \right) \right\}.$$

By Lemma 9,

$$\begin{aligned} (\psi, e_D^{\{K\}}) &= \sum_{k=1}^K \sum_{i=1}^p \left\{ R_i \left(\tilde{U}_i^{\{k\}}, \phi_i^{\{k\}} \right) \right. \\ &\quad \left. - \tau \sum_{m=1}^{k-1} \sum_{j=1}^p a_{ij} \left(e_{W,j}^{\{m\}}, \phi_i^{\{k\}} \right) + \tau \sum_{j=1}^p \sum_{l=k+1}^K a_{ij} \left(e_{W,i}^{\{k\}}, \phi_j^{\{l\}} \right) \right\}. \end{aligned}$$

Application of Galerkin orthogonality, similar to its use in the proof in Sect. 6.2.3, leads to

$$\begin{aligned} (\psi, e_D^{\{K\}}) &= \sum_{k=1}^K \sum_{i=1}^p \left\{ R_i \left(\tilde{U}_i^{\{k\}}, \phi_i^{\{k\}} - \pi_i \phi_i^{\{k\}} \right) - \tau \sum_{m=1}^{k-1} \sum_{j=1}^p a_{ij} \left(e_{W,j}^{\{m\}}, \phi_i^{\{k\}} \right) \right. \\ &\quad \left. + \tau \sum_{j=1}^p \sum_{l=k+1}^K a_{ij} \left(e_{W,i}^{\{k\}}, \phi_j^{\{l\}} \right) \right\}. \end{aligned}$$

The result follows if

$$\sum_{k=1}^K \sum_{j=1}^p \sum_{m=1}^{k-1} \sum_{i=1}^p a_{ij} \left(e_{W,i}^{\{m\}}, \phi_j^{\{k\}} \right) = \sum_{k=1}^K \sum_{i=1}^p \sum_{j=1}^p \sum_{l=k+1}^K a_{ij} \left(e_{W,i}^{\{k\}}, \phi_j^{\{l\}} \right),$$

where we interchanged the i and j loop indices on the left hand side. This follows if

$$\sum_{k=1}^K \sum_{m=1}^{k-1} a_{ij} \left(e_{W,i}^{\{m\}}, \phi_j^{\{k\}} \right) = \sum_{k=1}^K \sum_{l=k+1}^K a_{ij} \left(e_{W,i}^{\{k\}}, \phi_j^{\{l\}} \right). \quad (67)$$

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 $A_{k,m} = a_{ij} \left(e_{W,i}^{\{m\}}, \phi_j^{\{k\}} \right)$ for $m < k$. Then the left hand side of (67) is the sum of the entries of A by first summing each row while the right hand side of (67) is the sum of the entries of A by first summing each column. \square

7 Conclusions and future directions

We develop an adjoint based a posteriori error analysis to evaluate the 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 1” 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 1 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 2” solution in terms of the localized refinement of the finite element mesh and the choices of overlap and number of iterations. Only very simple refinement strategies were employed here. A number of more sophisticated refinement strategies suggest themselves and are worthy of study, but the interaction between discretization and iteration errors can be subtle and advanced refinement strategies remain a topic for future research.

The adjoint based analysis in this article has focused exclusively on linear problems. Adjoint based analysis can be extended to nonlinear problems, see [22,34]. 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. In combination with earlier work on parallel methods for initial value problems [11], the current analysis should enable the development of an a posteriori analysis for a numerical method that is parallel in both space and time. Such an analysis would again enable an efficient two stage solution approach, using the distribution of various sources of error estimated from an initial coarse solution to inform the discretization choices for a second “production” computation.

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