

# On the Time-domain Decomposition of Parabolic Optimal Control Problems

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## 1 Introduction

The efficient solution of optimal control problems under partial differential equation (PDE) constraints has become an active area of research in the past decade. In this paper, we consider an optimal control problem where the constraint is a large system of linear ordinary differential equations (ODEs) arising from the semi-discretization of a linear PDE in space:

$$\partial_t \mathbf{y} + \mathbf{A}\mathbf{y}(t) = \mathbf{B}\mathbf{u}(t) + \mathbf{f}(t), \quad t \in (0, T), \quad (1a)$$

$$\mathbf{y}(0) = \mathbf{y}_0. \quad (1b)$$

The goal is to find a control  $\mathbf{u}$  that minimizes the objective functional

$$F(\mathbf{u}) = \frac{1}{2} \int_0^T \|\mathbf{u}(t)\|^2 dt + \frac{\alpha_1}{2} \int_0^T \|C\mathbf{y} - \hat{\mathbf{y}}\|^2 dt + \frac{\alpha_2}{2} \|D\mathbf{y}(T) - \hat{\mathbf{y}}_T\|^2. \quad (2)$$

In the above,  $\hat{\mathbf{y}} = \hat{\mathbf{y}}(t)$  and  $\hat{\mathbf{y}}_T$  are the target trajectory and target state, and the functions  $\mathbf{u}$  and  $\mathbf{y} = \mathbf{y}(t, \mathbf{u})$  are called the control and the state, respectively. (For the purpose of analysis, we will use an appropriate change of variables to subsume any mass matrices that appear into the matrices  $A$ ,  $B$ ,  $C$  and  $D$ .) We will focus on the case where there are no control or state constraints, and where the governing equation is parabolic, i.e., when  $A$  is positive semi-definite, but not necessarily symmetric.

A formulation similar to the above has been used for a variety of problems where the goal is to drive a mechanical system to a desired state while minimizing the cost: it has been used for the control of fluid flow modelled by the Navier-Stokes equations [4, 23], boundary control problems for the wave equation [14] and quantum control (see [18] and references therein).

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Recently, medical applications have also been proposed, more specifically in the optimized administration of radiotherapy to control tumour growth [5].

For problems with no control or state constraints, a Lagrange-multiplier argument shows that the optimal control satisfies, in addition to the forward differential equation (1), the adjoint final value problem

$$\partial_t \boldsymbol{\lambda} - A^\top \boldsymbol{\lambda} = \alpha_1 C^\top (C\mathbf{y} - \hat{\mathbf{y}}), \quad (3a)$$

$$\boldsymbol{\lambda}(T) + \alpha_2 D^\top D\mathbf{y}(T) = \alpha_2 D^\top \hat{\mathbf{y}}_T, \quad (3b)$$

where  $\boldsymbol{\lambda}$ , the adjoint state, satisfies  $\mathbf{u} = B^\top \boldsymbol{\lambda}$ . Together with (1), this leads to a coupled forward-backward ODE system that must be further discretized in time and solved. Alternatively, one can discretize (1) and (2) in time and solve the resulting discrete saddle-point system. Note that the two approaches do not always “commute”, even if one chooses compatible time discretizations for (1a) and (3), see [6, 11]. Regardless of the approach taken, the exceedingly large size of the resulting linear system strongly motivates the use of parallel solution strategies. In this paper, we only consider the semi-discrete ODE system; the effect of discretization in time will be studied in a future paper.

There has been much progress in recent years in the development of effective preconditioners for saddle-point systems that arise from PDE-constrained optimal control problems; we only mention two classes of such methods. The first, known as the *all-at-once approach*, uses block preconditioners that are known to be effective for saddle-point systems. Because of its large size, the saddle-point matrix is not formed explicitly; instead, one performs the matrix-vector multiplication and preconditioning steps by solving forward and backward problems similar to (1) and (3). The latter steps can be parallelized in time using e.g. parareal [15] or parabolic multigrid [13, 10], or in space by domain decomposition or multigrid methods. We refer the reader to [21, 20], as well as to [22] for an approach in the infinite-dimensional setting which also works for problems with control constraints.

A different idea is to apply parallel methods directly to the optimal control problem itself. One such approach, known as the collective smoothing multigrid (CSMG) scheme, applies multigrid smoothing and coarsening to the coupled system and is analyzed in [3]. One can also adapt parareal to solve optimal control problems directly, see [18, 19, 17, 9]. Another approach, which arises from the multiple shooting philosophy, is to create smaller problems by subdividing the time horizon. The problem then consists of finding the intermediate state and adjoint variables that achieve both local optimality on each sub-interval and consistency across neighbouring sub-intervals. The smaller local problems can then be solved independently, and in parallel. This idea has been used in [12] to derive a block preconditioner for parabolic control problems, and in [14] to obtain a method with Robin-type consistency conditions in the context of wave equations. In [1], the authors consider an additive Schwarz preconditioner that uses Dirichlet interface conditions in the state and adjoint variables across overlapping sub-intervals.

## 2 Optimized Schwarz Methods in Time for Control

In [8], we introduced a time-domain decomposition method inspired by the Robin-type interface conditions used in optimized Schwarz methods (OSM) for elliptic problems. In this paper, we consider the natural extension to problems with non-trivial observation and control operators, namely

1. For  $k = 1, 2, \dots$ , solve in parallel for  $j = 1, 2$

$$\partial_t \mathbf{y}_j^k + A \mathbf{y}_j^k = B \mathbf{u}_j^k + \mathbf{f}(t), \quad \partial_t \boldsymbol{\lambda}_j^k - A^\top \boldsymbol{\lambda}_j^k = \alpha_1 C^\top (C \mathbf{y}_j^k - \hat{\mathbf{y}}) \quad (4)$$

on  $I_1 = (0, \beta)$  and  $I_2 = (\beta, T)$ , subject to  $\mathbf{u}_j^k = B^\top \boldsymbol{\lambda}_j^k$  and the initial and final conditions

$$\text{For } I_1: \quad \mathbf{y}_1^k(0) = \mathbf{y}_0, \quad \boldsymbol{\lambda}_1^k(\beta) + p \mathbf{y}_1^k(\beta) = \mathbf{h}^{k-1}, \quad (5)$$

$$\text{For } I_2: \quad \mathbf{y}_2^k(\beta) - q \boldsymbol{\lambda}_2^k(\beta) = \mathbf{g}^{k-1}, \quad \boldsymbol{\lambda}_2^k(T) + \alpha_2 D^\top D \mathbf{y}_2^k(T) = \alpha_2 D^\top \hat{\mathbf{y}}_T. \quad (6)$$

2. Update traces:

$$\mathbf{g}^k = \mathbf{y}_1^k(\beta) - q \boldsymbol{\lambda}_1^k(\beta), \quad \mathbf{h}^k = \boldsymbol{\lambda}_2^k(\beta) + p \mathbf{y}_2^k(\beta). \quad (7)$$

The parameters  $p$  and  $q$  are chosen to optimize convergence. In [8], the method is analyzed by assuming  $B = C = I$ ,  $D = 0$  and that  $A$  is symmetric. This allows us to diagonalize  $A$  and obtain explicit formulas for the contraction factors, but the analysis no longer works when  $A$  is non-symmetric. In this paper, we show a different method, based on energy estimates, which allows one to derive optimal parameters for non-symmetric operators  $A$ .

In terms of implementation, each iteration of the method (4)–(7) requires the solution of subdomain problems with Robin interface conditions. This may be done using any serial method, such as the all-at-once methods mentioned in Section 1. In the numerical experiments in Section 4, we use a Krylov-accelerated iteration based on shooting methods, which are easy to implement and naturally applicable to problems with optimized transmission conditions in time. For example, to solve the local problem on  $I_2$ , we consider the mapping  $\mathcal{P}_2(\mathbf{y}_\beta, \mathbf{u}) = [\mathbf{y}_\beta - q \boldsymbol{\lambda}(\beta) - \mathbf{g}^{k-1}, \mathbf{u} - B^\top \boldsymbol{\lambda}]$ , where the inputs are the initial state  $\mathbf{y}_\beta$  and the control function  $\mathbf{u} = \mathbf{u}(t)$ ,  $t \in I_2$ , and  $\boldsymbol{\lambda}$  is calculated by integrating  $\mathbf{y}$  forward in time, obtaining  $\boldsymbol{\lambda}(T)$  via the final condition in (6), and integrating  $\boldsymbol{\lambda}$  backward in time. Because the differential equations are linear, there exists a linear operator  $\mathcal{K}_2$  such that  $\mathcal{P}_2(\mathbf{y}_\beta, \mathbf{u}) = \mathcal{K}_2(\mathbf{y}_\beta, \mathbf{u}) + \mathbf{r}_0$  with  $\mathbf{r}_0 = \mathcal{P}_2(0, 0)$ . To calculate the solution, which satisfies  $\mathcal{P}_2(\mathbf{y}_\beta, \mathbf{u}) = 0$ , it suffices to solve  $\mathcal{K}_2(\mathbf{y}_\beta, \mathbf{u}) = -\mathbf{r}_0$  using a Krylov subspace method such as GMRES. The preconditioning of such systems is an important topic that will be addressed in a future paper. Nonetheless, we have observed in our experiments that the local solves converge within about 20 GMRES iterations, even without preconditioning.

## 2.1 Energy Estimates

To illustrate the technique for obtaining error estimates, we first consider the simple case of distributed control and observation with no target state (i.e.,  $B = C = I$ ,  $\alpha_2 = 0$ ). By linearity, it suffices to consider the problem with zero data (i.e.  $\mathbf{f}(t)$ ,  $\mathbf{y}_0$ ,  $\hat{\mathbf{y}}$  and  $\hat{\mathbf{y}}_T$  are all taken to be zero) and study how the approximate solution converges to zero. To derive an energy estimate for the first subdomain  $\Omega \times I_1$ , where  $I_1 = (0, \beta)$ , we introduce the auxiliary variables  $\mathbf{z}_1^k := \mathbf{y}_1^k + r\boldsymbol{\lambda}_1^k$ ,  $\boldsymbol{\mu}_1^k := \boldsymbol{\lambda}_1^k - s\mathbf{y}_1^k$  with  $r, s > 0$ . Note that the parameters  $r$  and  $s$  are not the same as the optimization parameters  $p$  and  $q$  and do not appear in the algorithm; they are introduced for analysis purposes only and must be chosen based on a given  $(p, q)$  pair. We now let  $H$  and  $S$  be the symmetric and skew-symmetric parts of  $A$ , such that  $A = H + S$ , and rewrite the problem (4) for subdomain  $I_1$  in terms of  $\mathbf{z}_1^k$  and  $\boldsymbol{\mu}_1^k$  to get

$$\begin{cases} \partial_t \mathbf{z}_1^k + \frac{1}{1+rs} [(1-rs)H + (1+rs)S - (\alpha_1 r + s)I] \mathbf{z}_1^k \\ \quad + \frac{1}{1+rs} [(\alpha_1 r^2 - 1)I - 2rH] \boldsymbol{\mu}_1^k = 0, \\ \partial_t \boldsymbol{\mu}_1^k + \frac{1}{1+rs} [(s^2 - \alpha_1)I - 2sH] \mathbf{z}_1^k \\ \quad + \frac{1}{1+rs} [(\alpha_1 r + s)I - (1-rs)H + (1+rs)S] \boldsymbol{\mu}_1^k = 0. \end{cases}$$

Note that the matrix multiplying  $\mathbf{z}_1^k$  in the first equation is exactly the negative transpose of the matrix multiplying  $\boldsymbol{\mu}_1^k$  in the second equation. This means if we multiply the first and second equations by  $(\boldsymbol{\mu}_1^k)^\top$  and  $(\mathbf{z}_1^k)^\top$  and add the results, the mixed terms cancel. After integrating over  $(0, \beta)$ , we obtain the energy identity

$$\begin{aligned} 0 = & \boldsymbol{\mu}_1^k(\beta)^\top \mathbf{z}_1^k(\beta) - \boldsymbol{\mu}_1^k(0)^\top \mathbf{z}_1^k(0) + \frac{1}{1+rs} \int_0^\beta (\boldsymbol{\mu}_1^k)^\top (\alpha_1 r^2 - 2rH - 1) \boldsymbol{\mu}_1^k \\ & + \frac{1}{1+rs} \int_0^\beta (\mathbf{z}_1^k)^\top (s^2 - 2sH - \alpha_1) \mathbf{z}_1^k \end{aligned} \quad (8)$$

Similarly, for the second subdomain  $I_2$ , we obtain

$$\begin{aligned} 0 = & \boldsymbol{\mu}_2^k(T)^\top \mathbf{z}_2^k(T) - \boldsymbol{\mu}_2^k(\beta)^\top \mathbf{z}_2^k(\beta) + \frac{1}{1+\hat{r}\hat{s}} \int_\beta^T (\boldsymbol{\mu}_2^k)^\top (\alpha_1 \hat{r}^2 - 2\hat{r}H - 1) \boldsymbol{\mu}_2^k \\ & + \frac{1}{1+\hat{r}\hat{s}} \int_\beta^T (\mathbf{z}_2^k)^\top (\hat{s}^2 - 2\hat{s}H - \alpha_1) \mathbf{z}_2^k, \end{aligned} \quad (9)$$

where we used the auxiliary variables  $\mathbf{z}_2^k := \mathbf{y}_2^k + \hat{r}\boldsymbol{\lambda}_2^k$  and  $\boldsymbol{\mu}_2^k := \boldsymbol{\lambda}_2^k - \hat{s}\mathbf{y}_2^k$ , with  $\hat{r}, \hat{s}$  possibly different from  $r, s$ .

To mimic the energy argument of [16], we need to ensure that the boundary terms in (8), (9) correspond to differences of incoming and outgoing Robin traces, and that the integral terms never change signs. This motivates the following theorem.

**Theorem 1.** *Consider the optimized Schwarz method (4)–(7) with  $B = C = I$  and  $\alpha_2 = 0$ . Assume that*

- (i) *The parameters  $r, s, \hat{r}, \hat{s}$  are non-negative,*
- (ii) *The matrices  $(1 - \alpha_1 r^2)I + 2rH$ ,  $(1 - \alpha_1 \hat{r}^2)I + 2\hat{r}H$ ,  $(\alpha_1 - s^2)I + 2sH$ ,  $(\alpha_1 - \hat{s}^2)I + 2\hat{s}H$  are all positive definite,*
- (iii) *There exist  $c_1, c_2 > 0$  such that  $(\boldsymbol{\mu}_1^k)^\top \mathbf{z}_1^k = c_1 \|\boldsymbol{\lambda}_1^k + p\mathbf{y}_1^k\|^2 - c_2 \|\mathbf{y}_1^k - q\boldsymbol{\lambda}_1^k\|^2$ ,*
- (iv) *There exist  $\hat{c}_1, \hat{c}_2 > 0$  such that  $(\boldsymbol{\mu}_2^k)^\top \mathbf{z}_2^k = \hat{c}_1 \|\boldsymbol{\lambda}_2^k + p\mathbf{y}_2^k\|^2 - \hat{c}_2 \|\mathbf{y}_2^k - q\boldsymbol{\lambda}_2^k\|^2$ .*

*Then the method satisfies the two-step error estimates*

$$\|\mathbf{y}_1^k(\beta) - q\boldsymbol{\lambda}_1^k(\beta)\|^2 \leq \rho^2 \|\mathbf{y}_1^{k-2}(\beta) - q\boldsymbol{\lambda}_1^{k-2}(\beta)\|^2, \quad (10a)$$

$$\|\boldsymbol{\lambda}_2^k(\beta) + p\mathbf{y}_2^k(\beta)\|^2 \leq \rho^2 \|\boldsymbol{\lambda}_2^{k-2}(\beta) + p\mathbf{y}_2^{k-2}(\beta)\|^2, \quad (10b)$$

with  $\rho^2 = \frac{c_1 \hat{c}_2}{c_2 \hat{c}_1}$ . In particular, the method converges if  $\rho^2 < 1$ .

*Proof.* Consider the energies

$$E_1^k = \frac{1}{1 + rs} \int_0^\beta (\boldsymbol{\mu}_1^k)^\top (1 + 2rH - \alpha_1 r^2) \boldsymbol{\mu}_1^k + (\mathbf{z}_1^k)^\top (\alpha_1 + 2sH - s^2) \mathbf{z}_1^k,$$

$$E_2^k = \frac{1}{1 + \hat{r}\hat{s}} \int_\beta^T (\boldsymbol{\mu}_2^k)^\top (1 + 2\hat{r}H - \alpha_1 \hat{r}^2) \boldsymbol{\mu}_2^k + (\mathbf{z}_2^k)^\top (\alpha_1 + 2\hat{s}H - \hat{s}^2) \mathbf{z}_2^k,$$

which must be positive by Assumption (ii) unless  $\boldsymbol{\mu}_1^k = \mathbf{z}_1^k = 0$  or  $\boldsymbol{\mu}_2^k = \mathbf{z}_2^k = 0$ . The energy equality (8) can then be written as

$$\boldsymbol{\mu}_1^k(\beta)^\top \mathbf{z}_1^k(\beta) - \boldsymbol{\mu}_1^k(0)^\top \mathbf{z}_1^k(0) = E_1^k \geq 0.$$

Using Assumption (iii) and the definition of  $\boldsymbol{\mu}_1^k$  and  $\mathbf{z}_1^k$ , we get

$$c_1 \|\boldsymbol{\lambda}_1^k(\beta) + p\mathbf{y}_1^k(\beta)\|^2 - c_2 \|\mathbf{y}_1^k(\beta) - q\boldsymbol{\lambda}_1^k(\beta)\|^2 - (\boldsymbol{\lambda}_1^k(0) - s\mathbf{y}_1^k(0))^\top (\mathbf{y}_1^k(0) + r\boldsymbol{\lambda}_1^k(0)) = E_1^k.$$

Since  $\mathbf{y}_1^k(0) = 0$  by (5), we in fact have

$$c_1 \|\boldsymbol{\lambda}_1^k(\beta) + p\mathbf{y}_1^k(\beta)\|^2 - c_2 \|\mathbf{y}_1^k(\beta) - q\boldsymbol{\lambda}_1^k(\beta)\|^2 = E_1^k + r \|\boldsymbol{\lambda}_1^k(0)\|^2 \geq 0. \quad (11)$$

But the transmission conditions (7) imply

$$c_1 \|\boldsymbol{\lambda}_2^{k-1}(\beta) + p\mathbf{y}_2^{k-1}(\beta)\|^2 \geq c_2 \|\mathbf{y}_1^k(\beta) - q\boldsymbol{\lambda}_1^k(\beta)\|^2. \quad (12)$$

A similar calculation on subdomain  $I_2$ , using Assumptions (ii), (iv) and the fact that  $\boldsymbol{\lambda}_2^k(T) = 0$ , yields

$$\hat{c}_2 \|\mathbf{y}_2^k(\beta) - q\boldsymbol{\lambda}_2^k(\beta)\|^2 - \hat{c}_1 \|\boldsymbol{\lambda}_2^k(\beta) + p\mathbf{y}_2^k(\beta)\|^2 = E_2^k + \hat{s} \|\mathbf{y}_2^k(T)\|^2 \geq 0. \quad (13)$$

The transmission conditions (7) now imply that

$$\hat{c}_2 \|\mathbf{y}_1^{k-1}(\beta) - q\boldsymbol{\lambda}_1^{k-1}(\beta)\|^2 \geq \hat{c}_1 \|\boldsymbol{\lambda}_2^k(\beta) + p\mathbf{y}_2^k(\beta)\|^2. \quad (14)$$

Combining the inequalities (12) and (14) and shifting indices when necessary leads to the two-step error estimates (10a)–(10b). If  $\rho^2 < 1$ , then we have

$$\|\mathbf{y}_j^k(\beta) - q\boldsymbol{\lambda}_j^k(\beta)\| \rightarrow 0 \quad \text{and} \quad \|\boldsymbol{\lambda}_j^k(\beta) + p\mathbf{y}_j^k(\beta)\| \rightarrow 0, \quad j = 1, 2.$$

We thus conclude from (11) and (13) that  $E_j^k \rightarrow 0$  for  $j = 1, 2$ , which implies that  $\boldsymbol{\mu}_j^k$  and  $\mathbf{z}_j^k$  both go to zero. This in turn shows that the error in the forward and adjoint states  $\mathbf{y}_j^k$  and  $\boldsymbol{\lambda}_j^k$  converges to zero, as required.  $\square$

In order to prove convergence of the method for a given choice of optimized parameters  $p$  and  $q$ , we need to show that there exists a choice of  $r, s, \hat{r}, \hat{s}$  such that the assumptions in Theorem 1 are satisfied. This is in fact possible if we assume  $pq < 1$ , together with some mild assumptions on  $H$ . For a proof of the following theorem, see [7].

**Theorem 2.** *Let  $B = C = I$  and  $\alpha_2 = 0$  (no target state). Assume that  $H = \frac{1}{2}(A + A^\top)$  is positive semi-definite. If  $p, q \geq 0$  satisfy  $pq < 1$ , then the optimized Schwarz method (4)–(7) converges for any initial guess, provided at least one of  $p$  and  $q$  is non-zero. Moreover, if  $H$  is positive definite, then the method also converges for  $p = q = 0$ .*

## 2.2 Choice of Parameters and Convergence Rates

We now show how to choose the parameters  $p, q$  in order to minimize the contraction factor  $\rho$  in Theorem 1. First, if  $H$  is only assumed to be positive semidefinite, then Assumption (ii) is satisfied provided

$$0 \leq r, \hat{r} < 1/\sqrt{\alpha_1}, \quad 0 \leq s, \hat{s} < \sqrt{\alpha_1}. \quad (15)$$

Now Assumption (iii) says

$$\boldsymbol{\mu}_1^\top \mathbf{z}_1 = (\boldsymbol{\lambda}_1 - s\mathbf{y}_1)^\top (\mathbf{y}_1 + r\boldsymbol{\lambda}_1) = c_1 \|\boldsymbol{\lambda}_1 + p\mathbf{y}_1\|^2 - c_2 \|\mathbf{y}_1 - q\boldsymbol{\lambda}_1\|^2, \quad (16)$$

while Assumption (iv) gives a similar relation for  $\hat{r}$  and  $\hat{s}$ . Expanding and equating coefficients for  $\boldsymbol{\lambda}_1^\top \boldsymbol{\lambda}_1$  and  $\mathbf{y}_1^\top \mathbf{y}_1$  in (16) leads to the formulas

$$c_1 = \frac{r + q^2 s}{1 - p^2 q^2}, \quad c_2 = \frac{s + p^2 r}{1 - p^2 q^2}, \quad (17)$$

where the denominators are non-zero because  $pq < 1$ , as stated in Theorem 2. Equating coefficients for  $\lambda_1^\top \mathbf{y}_1$  leads to a compatibility condition between  $r$  and  $s$ :

$$s = \frac{-2pr + (1 - pq)}{2q + r(1 - pq)} \iff r = \frac{-2qs + (1 - pq)}{2p + s(1 - pq)}.$$

For a given pair of optimized parameters  $(p, q)$  such that  $pq < 1$ , there are many ways of choosing  $r$  (or, equivalently,  $s$ ); our task is to choose  $r$  to obtain the best estimate for the convergence factor  $\rho$ . Using the above expressions to eliminate either  $r$  or  $s$  from (17) gives

$$\frac{c_1}{c_2} = \frac{q^2 + 2qr + r^2}{1 - 2pr + p^2r^2} = \left( \frac{q + r}{1 - pr} \right)^2 = \left( \frac{1 - qs}{p + s} \right)^2. \quad (18)$$

After deriving a similar expression for  $\hat{c}_1/\hat{c}_2$ , we conclude that the contraction factor  $\rho$  is

$$\rho = \frac{q + r}{1 - pr} \cdot \frac{p + \hat{s}}{1 - q\hat{s}}. \quad (19)$$

**Theorem 3.** *Let  $B = C = I$  and  $\alpha_2 = 0$  (no target state). If  $H = \frac{1}{2}(A + A^\top)$  is positive semidefinite, then the contraction factor  $\rho$  in (19) is minimized for*

$$p = \frac{\sqrt{\alpha_1}}{\sqrt{2} + 1}, \quad q = \frac{1}{\sqrt{\alpha_1}(\sqrt{2} + 1)}. \quad (20)$$

For these parameters, the two-subdomain OSM converges with the contraction factor

$$\rho = 3 - 2\sqrt{2} \approx 0.1716.$$

*Proof.* Since  $r$  is a decreasing function of  $s$  (and vice versa), the contraction factor in (19) can be minimized by choosing the smallest possible  $r$  and  $\hat{s}$  for which the corresponding  $s$  and  $\hat{r}$  satisfy the upper bounds in (15). Thus, the best choices of  $r$  and  $\hat{s}$  are given by

$$r = \max \left\{ 0, \frac{-2q\sqrt{\alpha_1} + (1 - pq)}{2p + \sqrt{\alpha_1}(1 - pq)} \right\}, \quad \hat{s} = \max \left\{ 0, \frac{-2p + \sqrt{\alpha_1}(1 - pq)}{2q\sqrt{\alpha_1} + (1 - pq)} \right\}.$$

This leads to the following formula for the contraction factor,

$$\rho = \max \left\{ q, \frac{1 - q\sqrt{\alpha_1}}{p + \sqrt{\alpha_1}} \right\} \cdot \max \left\{ p, \frac{\sqrt{\alpha_1} - p}{q\sqrt{\alpha_1} + 1} \right\},$$

which must be minimized within the region  $\{(p, q) : p > 0, q > 0, pq < 1\}$ . A somewhat tedious analysis shows that the minimum occurs for the values of  $p$  and  $q$  shown in (20), with the contraction factor  $\rho = 3 - 2\sqrt{2}$ .  $\square$

*Remark.* Since the contraction estimate is independent of the mesh parameter  $h$  and valid for any positive semidefinite matrix  $H$ , the above result is robust with respect to spatial and temporal grid refinement.

### 3 More Convergence Results

We now present two convergence results that hold in more general settings. For a proof of these results, we refer to [7].

*Multiple Subdomains.* It is straightforward to generalize (4)–(7) to the case of many time intervals. Theorem 2 holds for the general case as well. The technique of energy estimates allows us to prove the following result regarding convergence in the multiple subdomain case:

**Theorem 4.** *Suppose  $B = C = I$ ,  $\alpha_2 = 0$ . If  $H = \frac{1}{2}(A + A^\top)$  is positive semi-definite and  $h_T$  is the length of the shortest time sub-interval, then the optimized Schwarz method (4)–(7) converges whenever  $pq < 1$  and  $p, q$  are not both zero. Moreover, the optimal parameter is given asymptotically by*

$$p_{\text{opt}} = \sqrt{\alpha_1} - \alpha_1^{2/3}(4h_T)^{1/3} + O(h_T^{2/3}), \quad q_{\text{opt}} = p_{\text{opt}}/\alpha_1,$$

for which we have the contraction factor

$$\rho_{\text{opt}} = 1 - 2h_T\sqrt{\alpha_1} + O((h_T\sqrt{\alpha_1})^{5/3}).$$

*Control and Observation Over a Subset.* Consider a problem with non-trivial control and observation matrices  $B$  and  $C$ , so that the forcing terms in (4) are restricted to parts of the domain that are controllable or observable. In this case, the quantities inside the integrals in (8) become

$$(\boldsymbol{\mu}_1^k)^\top (\alpha_1 r^2 C^\top C - 2rH - BB^\top) \boldsymbol{\mu}_1^k \quad \text{and} \quad (\mathbf{z}_1^k)^\top (s^2 BB^\top - 2sH - \alpha_1 C^\top C) \mathbf{z}_1^k,$$

both of which must be zero or negative for all  $\mathbf{z}_1^k$  and  $\boldsymbol{\mu}_1^k$  in order for the energy estimates to hold. This restricts the range of allowable parameters  $r$  that can be chosen to minimize the contraction factor in (19). Together with a similar criterion on  $s$ , we obtain the following theorem.

**Theorem 5.** *Let  $\alpha_2 = 0$  (no target state). Suppose that*

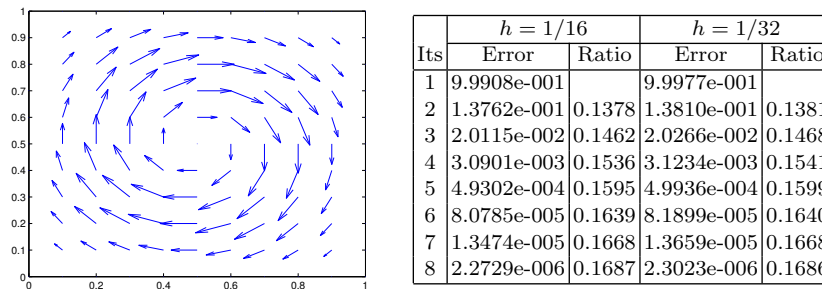
$$\ker(HB) \cap \ker(CB) = \{0\} \quad \text{and} \quad \ker(CH) \cap \ker(CB) = \{0\}.$$

*Then the method (4)–(7) with two subdomains converges if the non-negative parameters  $p$  and  $q$  are chosen such that  $pq < 1$  and  $(1 - pq)(1 - r^*s^*) < 2(pr^* + qs^*)$ , where*

$$r^* = \min_{\substack{\boldsymbol{\mu} \in \text{range}(C^\top) \\ \boldsymbol{\mu} \neq 0}} \frac{\boldsymbol{\mu}^\top H \boldsymbol{\mu}}{\alpha_1 \|C \boldsymbol{\mu}\|^2} + \sqrt{\left(\frac{\boldsymbol{\mu}^\top H \boldsymbol{\mu}}{\alpha_1 \|C \boldsymbol{\mu}\|^2}\right)^2 + \frac{\|B^\top \boldsymbol{\mu}\|^2}{\alpha_1 \|C \boldsymbol{\mu}\|^2}} > 0,$$

$$s^* = \min_{\substack{\mathbf{z} \in \text{range}(B) \\ \mathbf{z} \neq 0}} \frac{\mathbf{z}^\top H \mathbf{z}}{\|B^\top \mathbf{z}\|^2} + \sqrt{\left(\frac{\mathbf{z}^\top H \mathbf{z}}{\|B^\top \mathbf{z}\|^2}\right)^2 + \frac{\alpha_1 \|C \mathbf{z}\|^2}{\|B^\top \mathbf{z}\|^2}} > 0.$$





**Fig. 1** Left: velocity field used in the distributed control problem. Right: convergence of OSM for two time sub-intervals.

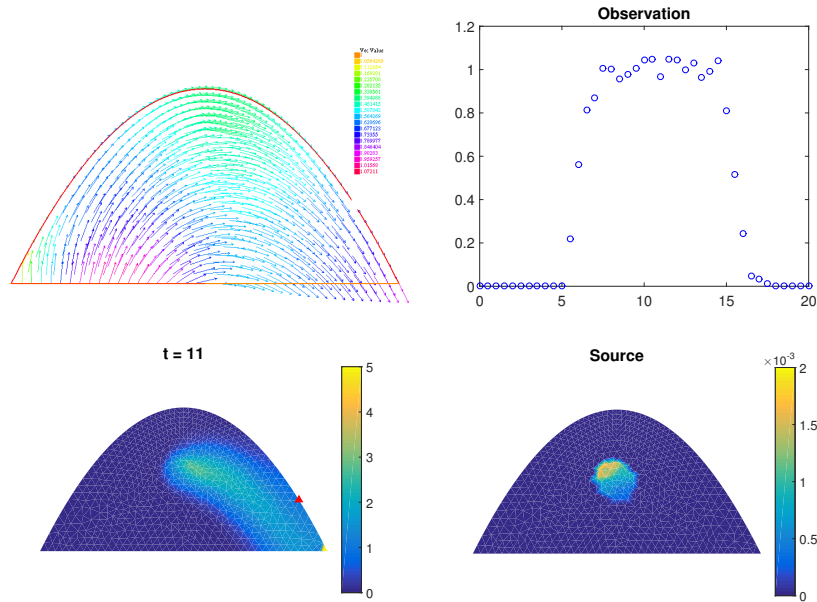
## 4 Numerical Experiments

*Distributed Control.* To illustrate Theorem 3, we consider the optimal control problem where the governing PDE is the two-dimensional advection-diffusion equation

$$y_t - \nabla \cdot (\nabla y + \mathbf{b}y) = u \quad \text{on } \Omega = (0, 1) \times (0, 1)$$

with  $\mathbf{b} = \sin \pi x_1 \sin \pi x_2 [x_2 - 0.5, 0.5 - x_1]^\top$  and no-flow conditions on  $\partial\Omega$ . The governing PDE is discretized using backward Euler in time and an upwind finite-difference discretization in space, with mesh parameters  $h = \frac{1}{16}$  and  $h = \frac{1}{32}$  respectively. The adjoint PDE is discretized using “forward” Euler, which is implicit because the adjoint runs backward in time. We solve the optimal control problem (2) over the time horizon  $(0, T)$  with  $T = 3$ ,  $\alpha_1 = 1$  and  $\alpha_2 = 0$ , i.e., we do not have a target state. The time window is subdivided into two intervals at  $\beta = 1$ . At the interface, we use Robin interface conditions with the optimized parameters suggested by Theorem 3, i.e.,  $p = q = \sqrt{2} - 1$ . The convergence history in Figure 1 shows that the error ratios approach the convergence factor of 0.1716, as predicted by Theorem 3.

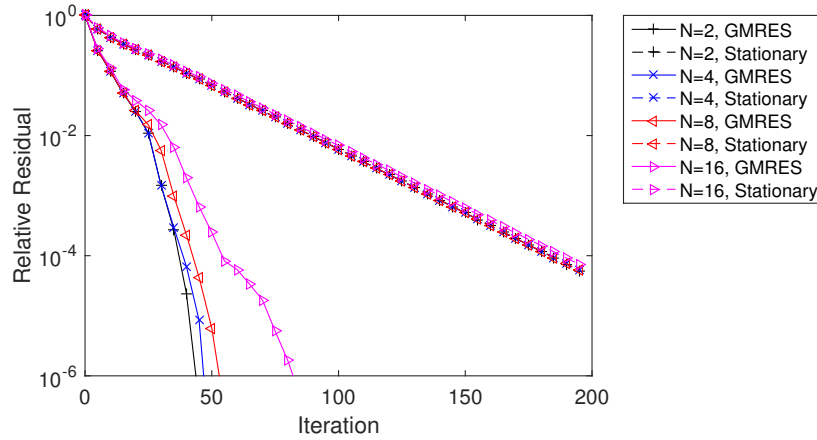
*Control and Observation Over Subsets.* For a more realistic example, we consider the problem of pollution tracking, where the goal is to estimate the rate at which a certain pollutant is released based on concentration readings elsewhere in the domain. The governing equation is the 2D advection-diffusion equation, where the domain is as shown in Figure 2. The flow field is computed by solving the Stokes equation, where the curved part of the domain is a no-flow boundary representing a shoreline, and the straight boundary contains in-flow and out-flow boundary conditions. The source of the pollution is a region near the centre of the domain, and we seek the rate of release that minimizes the discrepancy between the predicted and observed concentration at the point indicated by the red triangle on the curved boundary.



**Fig. 2** Top left: velocity field for the pollution tracking problem. Top right: concentrations observed at one point on the boundary. Bottom left: concentration at  $t = 11$  that best matches the observations at the boundary point indicated by the red triangle. Bottom right: release rate that yields the concentration to the left.

The advection-diffusion equation that models the concentration of pollutants is discretized using backward Euler in time and a finite volume method in space for unstructured grids, as presented in [2]. The resulting problem has 736 degrees of freedom in space, and the time interval of  $(0, T)$  with  $T = 20$  is split into 2, 4, 8 and 16 equal sub-intervals to test the optimized Schwarz method. Applying the minimization procedure in Theorem 3 to the bounds on  $r$  and  $s$  in Theorem 5, we determine the best parameters  $p$  and  $q$  to be 0.8563. We show in Figure 2 a snapshot of the concentration and source term that best match the observed concentration shown in the bottom right panel.

In Figure 3, we show the convergence of the OSM as a stand-alone solver and as a preconditioner used within GMRES. We see that the convergence of the stationary method depends only very weakly on the number of subdomains, even though Theorem 4 suggests that the number of iterations should scale like  $O(1/N)$ , where  $N$  is the number of subdomains. Nonetheless, when Krylov acceleration is used, we still see a moderate increase in the number of iterations as  $N$  increases. Thus, a coarse grid correction is most likely needed to ensure the scalability of the method. The design of a two-level method that incorporates coarse grid correction will be the subject of a future paper.



**Fig. 3** Convergence of the optimized Schwarz method applied to the pollution tracking problem.

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