On the Effect of Boundary Conditions on the
Scalability of Schwarz Methods

Gabriele Ciaramella and Luca Mechelli

1 Introduction

This work is concerned with convergence and weak scalability\(^1\) analysis of one-level parallel Schwarz method (PSM) and optimized Schwarz method (OSM) for the

\begin{equation}
- \Delta u = f \text{ in } \Omega, \quad u(a_1, y) = u(b_N, y) = 0 \quad y \in (0, 1),
\end{equation}

\begin{align*}
\mathcal{B}_b(u)(x) &= B_t(u)(x) = 0 \quad x \in (a_1, b_N),
\end{align*}

where \(\Omega\) is the domain depicted in Fig. 1, and \(\mathcal{B}_b\) and \(\mathcal{B}_t\) are either Dirichlet, or Neumann or Robin operators:

- **Dirichlet:** \(\mathcal{B}_b(u)(x) = u(0, x), \quad \mathcal{B}_t(u)(x) = u(1, x),\)
- **Neumann:** \(\mathcal{B}_b(u)(x) = \partial_y u(0, x), \quad \mathcal{B}_t(u)(x) = \partial_y u(1, x),\)
- **Robin:** \(\mathcal{B}_b(u)(x) = qu(0, x) - \partial_y u(0, x), \quad \mathcal{B}_t(u)(x) = qu(1, x) + \partial_y u(1, x).\)

Here, \(q > 0\) and the subscripts ‘\(b\)’ and ‘\(t\)’ stand for ‘bottom’ and ‘top’. As shown in Fig. 1, the domain \(\Omega\) is the union of subdomains \(\Omega_j, j = 1, \ldots, N,\) defined as \(\Omega_j := (a_j, b_j) \times (0, 1),\) where \(a_1 = 0, a_j = L + a_{j-1}\) for \(j = 2, \ldots, N + 1\) and \(b_j = a_{j+1} + 2\delta\) for \(j = 0, \ldots, N.\) Hence, the length of each subdomain is \(L + 2\delta\) and the length of the overlap is \(2\delta\) with \(\delta \in (0, L/2).\)

It is well known that one-level Schwarz methods are not weakly scalable, if the number of subdomains increases and the whole domain \(\Omega\) is fixed. However,
the recent work [2], published in the field of implicit solvation models used in computational chemistry, has drawn attention to the opposite case in which the number of subdomains increases, but their size remains unchanged, and, as a result, the size of the whole domain $\Omega$ increases. In this setting, weak scalability of PSM and OSM for (1) with Dirichlet boundary conditions is studied in [4, 3]. Scalability results for the PSM in case of more general geometries of the (sub)domains are presented in [5, 6, 7]. In these works, only external Dirichlet conditions are discussed and, in such a case, weak scalability is shown; see also [11] for a scalability analysis of the classical (alternating) Schwarz method. A short remark about the non-scalability in case of external Neumann conditions is given in [3]. Similar results have been recently presented in [1] for time-harmonic problems. Moreover, very similar results to the ones of [3] are obtained a few years later in [9]. The goal of this work is to study the effect of different (possibly mixed) external boundary conditions on convergence and scalability of PSM and OSM. In particular, we will show that only in the case of (both) external Neumann conditions at the top and the bottom of $\Omega$, PSM and OSM are not scalable. External Dirichlet conditions lead to the fastest convergence, while external Robin conditions lead to a convergence that depends heavily on the parameter $q$.

One-level PSM and OSM for the solution of (1) are

$$-\Delta u^n_j = f_j \text{ in } \Omega_j,$$

$$\mathcal{B}_b(u^n_j)(x) = \mathcal{B}_t(u^n_j)(x) = 0 \text{ for } x \in (a_1, b_N),$$

$$\mathcal{T}_\ell(u^n_j)(a_j) = \mathcal{T}_r(u^n_{j-1})(a_j), \quad \mathcal{T}_r(u^n_j)(b_j) = \mathcal{T}_r(u^n_{j+1})(b_j),$$

for $j = 1, \ldots, N$, where $\mathcal{T}_\ell$ and $\mathcal{T}_r$ are Dirichlet trace operators,

$$\mathcal{T}_\ell(u^n_j)(a_j) = u^n_j(a_j, y) \text{ and } \mathcal{T}_r(u^n_j)(b_j) = u^n_j(b_j, y),$$

for the PSM, and Robin trace operators,

$$\mathcal{T}_\ell(u^n_j)(a_j) = pu^n_j(a_j, y) - \partial_x u^n_j(a_j, y) \text{ and } \mathcal{T}_r(u^n_j)(b_j) = pu^n_j(b_j, y) + \partial_x u^n_j(b_j, y),$$

with $p > 0$ for the OSM. The subscript ‘$\ell$’ and ‘$r$’ stand for ‘left’ and ‘right’. For $j = 1$ the condition at $a_1$ must be replaced by $u^n_1(a_1, y) = 0$ and for $j = N$ the condition at $b_N$ must be replaced by $u^n_N(b_N, y) = 0$. In this paper, ‘external conditions’ and
where $q > 0$ and 'D', 'R' and 'N' stand for 'Dirichlet', 'Robin' and 'Neumann'. For all these six cases the eigenvalue problem \( (5) \) is solved by orthonormal (in $L^2(0,1)$) Fourier basis functions.

**Theorem 1** (Eigenpairs of the Laplace operator)

Let $q > 0$. The eigenproblems \( (5) \) with the above external conditions are solved by the non-trivial eigenpairs $(\varphi_k, \lambda_k)$ given by

(DD) $\varphi_k(y) = \sqrt{\frac{2}{\pi}} \sin(\pi ky), \lambda_k = \pi^2 k^2, k = 1, 2, \ldots$

(DR) $\varphi_k(y) = \sqrt{\frac{4\mu}{2\mu + \sin(2\mu)}} \sin(\mu ky), \lambda_k = \mu_k^2, k = 1, 2, \ldots$, where $\mu_k \in (k\pi - \pi/2, k\pi), k = 1, 2, \ldots$, are roots of $\hat{d}(x) := q \sin(x) + x \cos(x)$. Moreover, $\lim_{q \to 0} \mu_1(q) = \pi/2$ and $\lim_{q \to 0} \mu_1(q) = \pi$.

(DN) $\varphi_k(y) = \sqrt{\frac{2}{\pi}} \sin(\frac{2k+1}{2} \pi y), \lambda_k = \frac{(2k+1)^2}{4} \pi^2, k = 0, 1, 2, \ldots$

(RR) $\varphi_k(y) = \sqrt{\frac{4r_k}{2r_k + \sin(2r_k) + 4q \tau_k \sin(\tau_k)^2 + 2r_k^2 + 2q^2 r_k}} \left( q \sin(\tau_k y) + \tau_k \cos(\tau_k y) \right), \lambda_k = \tau_k^2, k = 1, 2, \ldots$, where $\tau_k \in (0, \pi), k = 1, 2, \ldots$, are roots of $\hat{d}(x) := 2qx \cos(x) + (q^2 - x^2) \sin(x)$. Moreover, $\lim_{q \to 0} \tau_1(q) = 0$ and $\lim_{q \to \infty} \tau_1(q) = \pi$.

(NR) $\varphi_k(y) = \sqrt{\frac{4v_k}{2v_k + \sin(2v_k)}} \cos(v_k y), \lambda_k = v_k^2, k = 1, 2, \ldots$, where $v_k \in ((k-1)\pi, (k - \frac{1}{2})\pi), k = 1, 2, \ldots$, are roots of $d(x) := x \sin(x) - q \cos(x)$. Moreover, $\lim_{q \to 0} v_1(q) = 0$ and $\lim_{q \to \infty} v_1(q) = \pi/2$. 

### 2 Laplace eigenpairs for mixed external conditions

Consider the 1D eigenvalue problem

\[
\varphi''(y) = -\lambda \varphi(y), \quad \text{for } y \in (0,1), \quad B_0(\varphi)(0) = B_0(\varphi)(1) = 0, \quad (5)
\]

and six pairs of boundary operators $(B_b, B_r)$:

- (DD) $B_b(\varphi)(0) = \varphi(0), \quad B_r(\varphi)(1) = \varphi(1)$
- (DR) $B_b(\varphi)(0) = \varphi(0), \quad B_r(\varphi)(1) = q\varphi(1) + \varphi'(1)$
- (DN) $B_b(\varphi)(0) = \varphi(0), \quad B_r(\varphi)(1) = \varphi'(1)$
- (RR) $B_b(\varphi)(0) = q\varphi(0) - \varphi'(0), \quad B_r(\varphi)(1) = q\varphi(1) + \varphi'(1)$
- (NR) $B_b(\varphi)(0) = \varphi'(0), \quad B_r(\varphi)(1) = q\varphi(1) + \varphi'(1)$
- (NN) $B_b(\varphi)(0) = \varphi'(0), \quad B_r(\varphi)(1) = \varphi'(1)$

We analyze convergence of PSM and OSM by a Fourier analysis in Section 3.
(NN) \( \varphi_k(y) = \sqrt{2} \cos(\pi k y), \lambda_k = \pi^2 k^2, k = 0, 1, 2, \ldots \)

**Proof** If we multiply (5) with \( \varphi \), integrate over [0, 1], and integrate by parts, we get
\[
\lambda \int_0^1 |\varphi(y)|^2 dy = \int_0^1 |\varphi'(y)|^2 dy - \varphi'(1)\varphi(1) + \varphi'(0)\varphi(0).
\]
Using any of the above external conditions (and that \( q > 0 \), for the Robin ones) one gets \( \lambda \geq 0 \). We refer to, e.g., [10, Section 4.1] for similar discussions. Now, all the cases can be proved by using the ansatz \( \varphi(y) = A \cos(\sqrt{\lambda} y) + B \sin(\sqrt{\lambda} y) \), which clearly satisfies (5), and computing, e.g., \( A \) and \( \lambda \) in such a way that \( \varphi(y) \) satisfies the two external conditions and \( B \) as a normalization factor. \( \square \)

The coefficients \( \nu_1, \mu_1 \) and \( \tau_1 \) as functions of \( q \) are shown in Fig. 2 (left), where we can observe that \( \nu_1(q) < \frac{\pi}{2} < \mu_1(q) < \pi \) and \( 0 < \tau_1(q) < \pi \), and that the maps \( q \mapsto \nu_1(q), q \mapsto \mu_1(q) \) and \( q \mapsto \tau_1(q) \) increase monotonically and approach, respectively, \( \frac{\pi}{2} \) and \( \pi \) as \( q \to \infty \). Hence, by taking the limit \( q \to 0 \), one can pass from the conditions (DR), (RR) and (NR) to (DN), (NN) and (NN), respectively. Similarly, by taking the limit \( q \to \infty \), the conditions (DR), (RR) and (NR) become (DD), (DD) and (DN), respectively.

3 Convergence and scalability

Consider the Schwarz method (2) and any pair \( (\mathcal{B}_b, \mathcal{B}_r) \) of operators as in Section 2. The Fourier expansions of \( u^n_j(x, y), j = 1, \ldots, N, \) are
\[
u_j^T(x, y) = \sum_k \tilde{u}_j^T(x, \lambda_k) \varphi_k(y), \tag{6}
\]
where the sum is over \( k = 1, 2, \ldots \) for (DD), (DR), (RR) and (NR), and over \( k = 0, 1, 2, \ldots \) for (DN) and (NN). The functions \( \varphi_k \) depend on the external boundary conditions and are the ones obtained in Theorem 1. The Fourier coefficients \( \tilde{u}_j^T(x, \lambda_k) \) satisfy\(^2\)
\[^2\] Notice that the procedure to obtain (7) is standard. We refer to, e.g., [10] for more details and examples.
On the Effect of Boundary Conditions on the Scalability of Schwarz Methods

\[
-\partial_{xx}u^n_j(x,\lambda_k) + \lambda_k \partial_x u^n_j(x,\lambda_k) = \bar{f}_j(x,\lambda_k) \text{ in } (a_j, b_j),
\]

\[
T_T(u^n_j(\cdot,\lambda_k))(a_j) = T_T(u^{n-1}_{j-1}(\cdot,\lambda_k))(a_j),
\]

\[
T_T(u^n_j(\cdot,\lambda_k))(b_j) = T_T(u^{n-1}_{j+1}(\cdot,\lambda_k))(b_j),
\]

(7)

for \( j = 1, \ldots, N \). For \( j = 1 \), the condition at \( a_1 \) must be replaced by \( u^n_1(a_1) = 0 \) and for \( j = N \) the condition at \( b_N \) must be replaced by \( u^n_N(b_N) = 0 \). If the operators \( T_T \) and \( T_T \) correspond to Dirichlet conditions (see (3)), then (7) is a PSM. If they correspond to Robin conditions (see (4)), then (7) is an OSM. The convergence of the iteration (7) is analyzed in Theorem 2.

**Theorem 2 (Convergence of Schwarz methods in Fourier space)**

The contraction factors of the Schwarz methods (7) are bounded by

\[
\rho(\lambda_k, \delta) = \frac{\kappa_{\lambda, \delta}^2 + e^{L_4}}{e^{2\lambda_4} + e^{L_4} + 1}.
\]

Moreover, it holds that \( \rho(\lambda_k, \delta) \in [0, 1] \) with \( \rho(0, 0) = 1 \) (independently of \( N \)), and that \( \lambda \mapsto \rho(\lambda, \delta) \) is strictly monotonically decreasing.

**Proof** The Dirichlet case follows from [4, Lemma 2 and Theorem 3]. See also [3, Lemma 2 and Theorem 1]. We focus here on the Robin case. From Theorem 3 in [3] and the corresponding proof we have that the contraction factor of the OSM is bounded by \( \max\{\phi(\lambda, \delta, p), |\zeta(\lambda, \delta, p)|\} \) where

\[
\phi(\lambda, \delta, p) := \frac{(\lambda + p)^2 e^{2\delta L} - (\lambda - p)^2 e^{-2\delta L} + (\lambda + p)(\lambda - p)(e^{L_4} - e^{-L_4})}{(\lambda + p)^2 e^{2\lambda_4} + (\lambda - p)^2 e^{-2\lambda_4}} \geq 0,
\]

\[
\zeta(\lambda, \delta, p) := \frac{(\lambda + p)^2 e^{-2\lambda_4} + (\lambda - p)^2 e^{2\lambda_4}}{(\lambda + p)^2 e^{2\lambda_4} + (\lambda - p)^2 e^{-2\lambda_4}},
\]

with \( \phi(\lambda, \delta, p) \leq \phi(\lambda, \delta, 0) = \lim_{p \to 0} \phi(\lambda, \delta, p) = \frac{e^{2\delta L} - e^{-2\delta L}}{e^{L_4} + e^{-L_4}} \) for all \( \lambda \geq 0 \) and \( \delta > 0 \). If we compute the derivative of \( \lambda \mapsto \phi(\lambda, \delta, 0) \) we get

\[
\partial_\lambda \phi(\lambda, \delta, 0) = -\frac{L(\lambda L_4 + 1) - e^{2\lambda_4}}{(e^{2\lambda_4} + 1)^2} + 2\delta(e^{2\lambda_4 + 2\lambda_4} - e^{2\lambda_4}),
\]

which is negative for any \( \lambda \geq 0 \) and \( \delta > 0 \). Thus, \( \lambda \mapsto \phi(\lambda, \delta, 0) \) is strictly monotonically decreasing. Let us now study the function \( \zeta(\lambda, \delta, p) \). Direct calculations reveal that \( \partial_\lambda \zeta(\lambda, \delta, p) = -\frac{L(\lambda L_4 + 1)^2 - e^{2\lambda_4}}{(e^{2\lambda_4} + 1)^2} \), which is negative for any \( \lambda > 0 \) and \( \delta > 0 \), and \( \zeta(\lambda, \delta, 0) = \frac{e^{2\lambda_4 L_4} - e^{-2\lambda_4 L_4}}{e^{L_4 + 2\lambda_4} + e^{-L_4 - 2\lambda_4}} > 0 \) and \( \lim_{p \to 0} \zeta(\lambda, \delta, p) = \frac{e^{2\lambda_4 L_4} - e^{-2\lambda_4 L_4}}{e^{2\lambda_4 + 2\lambda_4} + e^{-2\lambda_4}} < 0 \) for any \( \lambda \geq 0 \) and \( \delta > 0 \). These observations imply that \( p \mapsto \zeta(\lambda, \delta, p) \) is strictly monotonically decreasing and attains its maximum at \( p = 0 \). Finally, a direct comparison shows that \( \phi(\lambda, \delta, 0) \geq \zeta(\lambda, \delta, 0) \) \( \lim_{p \to 0} |\zeta(\lambda, \delta, p)| = |\zeta(\lambda, \delta, 0)| \) and the result follows, because \( \phi(\lambda, \delta, 0) = \frac{e^{2\delta L} - e^{-2\delta L}}{e^{L_4} + e^{-L_4}} = e^{2\delta L} e^{-2\delta L} \).

\[\square\]

3 The contraction factor for (7) (corresponding to the \( k \)-th Fourier component) is the spectral radius of the Schwarz iteration matrix; see [4, 3].
Theorem 2 gives the same bound (8) for the convergence factors of PSM and OSM. This fact is not surprising. First, it is well known that OSM converges faster than PSM for $\delta > 0$. Hence, a convergence bound for the PSM is a valid bound also for the OSM. Second, in the above proof the convergence bound for the OSM is obtained for $p \to \infty$, which corresponds to passing from Robin transmission conditions to Dirichlet transmission conditions. The bound (8) is based on the ones obtained in [4, 3]. These are quite sharp for large values of $N$; see, e.g., [3, Fig. 4 and Fig. 5].

We can now prove our main convergence result, which allows us to study convergence and scalability of PSM and OSM for all the external conditions considered in Section 2.

**Theorem 3 (Convergence of PSM and OSM)**

The contraction factors (in the $L^2$ norm) of PSM and OSM for the solution to (1) are bounded by

- (DD) $\rho_{DD}(\delta) := \rho(\pi^2, \delta)$,
- (DR) $\rho_{DR}(\delta, q) := \rho(\mu_1(q)^2, \delta)$,
- (DN) $\rho_{DN}(\delta) := \rho(\pi^2/4, \delta)$,
- (RR) $\rho_{RR}(\delta, q) := \rho(\tau_1(q)^2, \delta)$,
- (NR) $\rho_{NR}(\delta, q) := \rho(v_1(q)^2, \delta)$,
- (NN) $\rho_{NN}(\delta) := \rho(0, \delta) = 1$,

where $q \in (0, \infty)$ and $\rho(\lambda, \delta)$ is defined in Theorem 2. Moreover, for any $\delta > 0$ we have that

- $\rho_{DD}(\delta) < \rho_{DR}(\delta, q) < \rho_{DN}(\delta) < \rho_{NR}(\delta, q) < \rho_{NN}(\delta) = 1$,  

- $\rho_{DD}(\delta) < \rho_{RR}(\delta, q) < \rho_{NN}(\delta) = 1$.  

**Proof** According to Theorem 2, the bounds of the Fourier contraction factor $\rho(\lambda, \delta)$ is monotonically decreasing in $\lambda$. Therefore, an upper bound for the convergence factor of PSM and OSM (in the $L^2$ norm) can be obtained by taking the maximum over the admissible Fourier frequencies $\lambda_k$ and invoking Parseval’s identity (see, e.g., [4]). Recalling Theorem 1, these maxima are attained at $\lambda_1 = \pi^2$ for (DD), $\lambda_1 = \mu_1^2$ for (DR), $\lambda_0 = \pi^2/4$ for (DN), $\lambda_1 = \tau_1^2$ for (RR), $\lambda_1 = \nu_1^2$ for (NR), and $\lambda_0 = 0$ for (NN). The inequalities (9) and (10) follow from the monotonicity $\lambda \mapsto \rho(\lambda, \delta)$ and the fact that $v_1(q) < \frac{\pi}{2} < \mu_1(q) < \pi$ and $\tau_1(q) \in (0, \pi)$. \qed

The inequalities (9) and (10) imply that the contraction factor is bounded, independently of $N$, by a constant strictly smaller than 1 for all the cases except (NN). In the case (NN), the first Fourier frequency is $\lambda_0 = 0$. Hence, the coefficients $\widehat{u}^n_j(x, \lambda_0)$ are generated by the 1D Schwarz method

$$-\partial_{xx}\widehat{u}^n_j(x, \lambda_0) = \widehat{f}_j(x, \lambda_0) \text{ in } (a_j, b_j),$$

$$T_\ell(\widehat{u}^n_j(\cdot, \lambda_0))(a_j) = T_\ell(\widehat{u}^n_{j-1}(\cdot, \lambda_0))(a_j),$$

$$T_\ell(\widehat{u}^n_j(\cdot, \lambda_0))(b_j) = T_\ell(\widehat{u}^n_{j+1}(\cdot, \lambda_0))(b_j),$$

which is known to be not scalable; see, e.g., [3, 8]. The scalability of PSM and OSM for different external conditions applied at the top and at the bottom of the domain is summarized in Table 1. Inequalities (9) and (10) lead to another interesting
observation. The contraction factors are clearly influenced by the external boundary conditions. Dirichlet conditions lead to faster convergence than Robin conditions, which in turn lead to faster convergence than Neumann conditions. For example, if one external condition is of the Dirichlet type, then PSM and OSM converge faster if the other condition is of the Dirichlet type and slower if this is of Robin and even slower for the Neumann type. The case (RR) is slightly different, because the corresponding convergence of PSM and OSM depends heavily on the Robin parameter $q$. The behavior of the bounds $\rho_{RR}(\delta, q)$, $\rho_{DR}(\delta, q)$ and $\rho_{NR}(\delta, q)$ with respect to $q$ is depicted in Fig. 2 (right), which shows the bounds discussed in Theorem 3 as functions of $q$ (recall that $\rho_{NN} = 1$). Here, we can observe that the inequalities (9) and (10) are satisfied and that

- As $q$ increases the Dirichlet part of the Robin external condition dominates. In addition, the bounds $\rho_{RR}$ and $\rho_{DR}$ decrease and approach $\rho_{DD}$ as $q \to \infty$. Similarly, $\rho_{NR}$ decreases and approaches $\rho_{DN}$.

- As $q$ decreases the Neumann part of the Robin external condition dominates. In addition, the bounds $\rho_{NR}$ and $\rho_{RR}$ decrease and approach $\rho_{NN} = 1$ as $q \to 0$. Similarly, $\rho_{DR}$ increases and approaches $\rho_{DN}$.

These observations lead to Tab. 1 (right), where we summarize the robustness of PSM and OSM with respect to the parameter $q$. The methods are robust with respect to $q$ only if one of the two external boundary conditions is of Dirichlet type. This is due to the fact that Robin conditions become Neumann conditions for $q \to 0$.

### 4 Numerical experiments

In this section, we test the scalability of PSM and OSM by numerical simulations. For this purpose, we run PSM and OSM for all the external boundary conditions discussed in this paper and measure the number of iterations required to reach a tolerance on the error of $10^{-6}$. To guarantee that the initial errors contain all frequencies, the methods are initialized with random initial guesses. In all cases, each subdomain is discretized with a uniform grid of size 90 interior points in direction $x$ and 50 interior points in direction $y$. The mesh size is $h = \frac{L}{51}$, with $L = 1$, and the overlap parameter is $\delta = 10h$. For the OSM the robin parameter is $p = 10$. The Robin parameter $q$ of the external Robin conditions is $q = 10$, and the (RR) case is also tested with $q = 0.1$. The results of our experiments are shown in Tab. 2 and confirm the theoretical results discussed in the previous sections.
Table 2: Number of iterations of PSM (left) and OSM (right) needed to reduce the norm of the error below a tolerance of $10^{-6}$ for increasing number $N$ of fixed-sized subdomains. The maximum number of allowed iterations is 401. This limit is only reached in the (NN) case, for which PSM and OSM are not scalable.

References