

1 **On the scalability of classical one-level domain-decomposition**  
2 **methods**

3 **F. Chaouqui**<sup>1</sup> · **G. Ciaramella**<sup>2</sup> · **M. J. Gander**<sup>1</sup> ·  
4 **T. Vanzan**<sup>1</sup>

5  
6 the date of receipt and acceptance should be inserted later

7 **Abstract** One-level domain decomposition methods are in general not scalable, and coarse  
8 corrections are needed to obtain scalability. It has however recently been observed in ap-  
9 plications in computational chemistry that the classical one-level parallel Schwarz method  
10 is surprisingly scalable for the solution of one- and two-dimensional chains of fixed-sized  
11 subdomains. We first review some of these recent scalability results of the classical one-level  
12 parallel Schwarz method, and then prove similar results for other classical one-level domain-  
13 decomposition methods, namely the optimized Schwarz method, the Dirichlet-Neumann  
14 method, and the Neumann-Neumann method. We show that the scalability of one-level do-  
15 main decomposition methods depends critically on the geometry of the domain decompo-  
16 sition and the boundary conditions imposed on the original problem. We illustrate all our  
17 results also with numerical experiments.

18 **Keywords** domain-decomposition methods; scalability; classical and optimized Schwarz  
19 methods; Dirichlet-Neumann method; Neumann-Neumann method; solvation model; chain  
20 of atoms; Laplace's equation.

21 **AMS Classification** 65N55, 65F10, 65N22, 70-08, 35J05, 35J57.

22 **1 Introduction**

23 Recent developments in physical and chemical applications are creating a large demand for  
24 numerical methods for the solution of complicated systems of equations, which are often  
25 used before rigorous numerical analysis results are available. Moreover, the nature of the  
26 applications makes such systems untreatable by sequential algorithms and generates the  
27 need of methods that are parallel in nature or that can be easily parallelized.

28 In the field of parallel methods an important role is played by the so-called “scalability  
29 property” of an algorithm. An algorithm is “strongly scalable”, if the acceleration generated  
30 by the parallelization scales proportionally with the number of processors that are used.  
31 For example if on 10 processors, a strongly scalable algorithm needs 10 seconds to solve

---

Work supported by ...

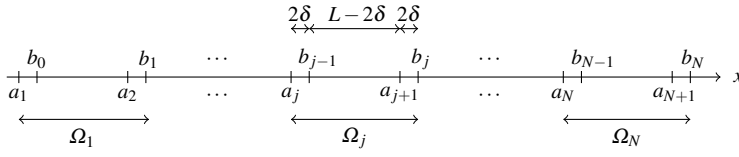
<sup>1</sup> Section de mathématiques, Université de Genève, 2-4 rue du Lièvre, Genève,

<sup>2</sup> Fachbereich Mathematik und Statistik, University of Constance, Germany.

the problem, it would need 1 second using 100 processors. Strong scalability is difficult to achieve, because eventually there is not enough work left to do for each processor and communication dominates, but it is possible up to some point, see for instance Table 1 in [30] and Table 3 in [23]. One therefore also talks about “weak scalability”, which means that one can solve a larger and larger problem with more and more processors in a fixed amount of time. For example, if a weakly scalable algorithm solves a problem with 100’000 unknowns in 10 seconds using 10 processors, it should be able to solve a problem with 1’000’000 unknowns in the same 10 seconds using 100 processors. In particular, a domain-decomposition method is said to be weakly scalable, if its rate of convergence does not deteriorate when the number of subdomains grows [40].

To analyze weak scalability, we study in this paper the contraction (or convergence) factor  $\rho$  of the algorithms, the convergence rate being  $-\log \rho$ , see [27, Section 11.2.5]. Thus if the contraction factor of a method does not deteriorate, also the convergence rate does not deteriorate and the method is weakly scalable. To explain now what the contraction factor  $\rho$  of a stationary iterative method is, we assume that it generates for iteration index  $0, 1, 2, \dots$  an error sequence  $\mathbf{e}^0, \mathbf{e}^1, \mathbf{e}^2, \dots$  converging geometrically in a given norm  $\|\cdot\|$ , that is  $\frac{\|\mathbf{e}^n\|}{\|\mathbf{e}^0\|} \leq \rho^n$ , and  $\rho$  is the associated contraction factor. Now, assume that the iterative procedure stops at a given tolerance  $\text{To1}$ , that is  $\frac{\|\mathbf{e}^n\|}{\|\mathbf{e}^0\|} \approx \text{To1}$ . By combining these two formulas we get  $\text{To1} \approx \frac{\|\mathbf{e}^n\|}{\|\mathbf{e}^0\|} \leq \rho^n$ , and estimate the number of iterations necessary to achieve  $\text{To1}$  as  $n \leq \frac{|\log \text{To1}|}{|\log \rho|}$ . If the contraction factor  $\rho$  of a domain decomposition method is uniformly bounded by a constant strictly less than one, independently of the number of subdomains  $N$ , then the method converges to a given tolerance with a number of iterations  $n$  that is independent of the number of subdomains  $N$ , and the method is thus weakly scalable: its convergence rate  $-\log \rho$  can not deteriorate when the number of subdomains grows. We study therefore in Sections 3,4,5 and 6 the contraction factors for different domain decomposition methods, and we provide a constant bound strictly less than one which is independent of the number of subdomains  $N$ , provided that size of the subdomains is fixed, which is a sufficient condition for the domain decomposition methods to be weakly scalable.

As a particular example of this weak-scalability behavior, we recall the new methodology that was recently presented in [3] and supported by [34,35]. Based on a physical approximation of solvation phenomena [1, 29, 41], the authors introduced a new formulation of the Schwarz domain-decomposition methods for the solution of solvation problems, where large molecular systems, given by chains of atoms, are involved. Each atom corresponds in this formulation to a subdomain, and the Schwarz methods are written in a boundary element form. The authors have observed in their numerical experiments the surprising result that the convergence of the iterative procedure without coarse correction is in many cases independent of the number of atoms and thus subdomains, which means that simple one-level Schwarz (alternating and parallel) methods for the solution of chains of particles are weakly scalable; no coarse correction seems to be necessary. On the other hand, it is well known that the convergence of Schwarz methods without coarse correction depends in general for elliptic problems on the number of subdomains, see for example [40]. The surprising scalability result of the classical one-level Schwarz method in the special case of a chain of atoms was recently explained using three different types of analysis: in [6], the authors used Fourier analysis for an approximate 2-dimensional model that describes a chain of atoms whose domains are approximated by rectangles; in [7], the maximum principle was used for more realistic 2-dimensional chains of atoms; in [8] the unusual scaling behavior was explained using variational methods. These scalability results represent exceptions to the classical Schwarz theory [40], which shows that one-level domain-decomposition



**Fig. 1** One-dimensional chain of  $N$  fixed-sized subdomains of length  $L + 2\delta$ . The overlap is  $2\delta$ .

80 methods are in general not scalable. Two-level domain-decomposition methods, i.e. domain-  
 81 decomposition methods with coarse corrections, attempt to reach this goal; see the seminal  
 82 contributions [37, 10], and [12] for FETI, and more generally the books [39, 38, 40] and refer-  
 83 ences therein. Coarse spaces were also developed for optimized Schwarz methods, see the  
 84 first contribution [11], and [17], which is based on the new idea of optimal coarse spaces and  
 85 their approximation from [16], see [19] for a general introduction. Optimal coarse spaces  
 86 lead to convergence in a finite number of iterations [4], i.e. the method becomes nilpotent,  
 87 and for certain decompositions and methods this is even possible without coarse space,  
 88 see [5]. Based on the optimal coarse space, optimized variants were developed in [18] for  
 89 restricted additive Schwarz, in [24] for additive Schwarz, and in [21, 20] for multiscale prob-  
 90 lems, including a condition number estimate.

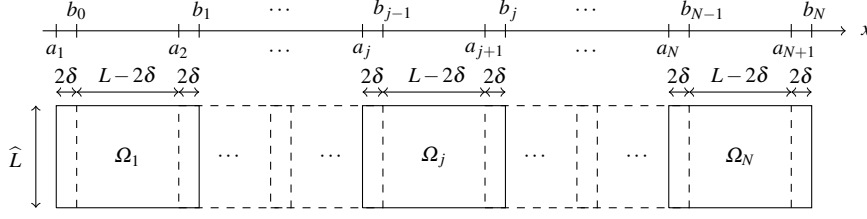
91 At this point it seems natural to ask: is it possible for other classical domain decompo-  
 92 sition methods to be scalable without coarse correction, like Dirichlet-Neumann methods,  
 93 Neumann-Neumann methods, and optimized Schwarz methods? Answering this question  
 94 is the main goal of this paper. We focus on the Laplace equation defined on one- and two-  
 95 dimensional chains of subdomains introduced in Section 2, because scalability depends on  
 96 the dimension and the boundary conditions. We then define the parallel Schwarz method for  
 97 the solution to these models in Section 3, and review the scalability results from [6]. In Sec-  
 98 tion 4, we prove that also optimized Schwarz methods have the same scalability properties,  
 99 and this even without overlap. Section 5 focuses on the scalability analysis of the Dirichlet-  
 100 Neumann method, and Section 6 on the Neumann-Neumann method. In all cases, we prove  
 101 that these one-level methods can be scalable for certain geometric situations and boundary  
 102 conditions. We illustrate our analysis with numerical experiments in Section 7.

## 103 2 Formulation of the problem: growing chains of fixed-sized subdomains

104 In this section, we define our model problems consisting of chains of  $N$  subdomains in  
 105 one and two spatial dimensions, which we will use to study classical one-level domain-  
 106 decomposition methods. In particular, we are interested in the behavior of these methods  
 107 when the number  $N$  of subdomains grows while their size is fixed.

108 We begin describing the one-dimensional problem. Consider the domain  $\Omega = (a_1, b_N)$   
 109 shown in Figure 1, where the two extrema are the first and the last elements of two sets of  
 110 points  $a_j$ , for  $j = 1, \dots, N + 1$ , and  $b_j$ , for  $j = 0, \dots, N$ , defined as  $a_j := (j - 1)L - \delta$  and  
 111  $b_j := jL + \delta$ . Therefore,  $a_j$  and  $b_j$  form a grid in  $\Omega$  and define the subdomains  $\Omega_j := (a_j, b_j)$   
 112 such that  $\Omega = \cup_{j=1}^N \Omega_j$ . The quantities  $L > 0$  and  $\delta > 0$  parametrize the dimension of each  
 113 subdomain  $\Omega_j$  and the overlap  $\Omega_j \cap \Omega_{j+1}$  whose length is  $2\delta$ . We are interested in the  
 114 solution to the problem

$$-\Delta u = f \text{ in } \Omega, u(a_1) = g_1, u(b_N) = g_N, \quad (1)$$



**Fig. 2** Two-dimensional chain of  $N$  rectangular fixed-sized subdomains.

115 where  $f$  is a sufficiently regular function and  $g_1, g_N \in \mathbb{R}$ . Problem (1) can be formulated as  
 116 follows: we introduce the function  $u_j$  as the restriction of  $u$  to  $\Omega_j$ . Hence  $u_j$  satisfies

$$\begin{aligned} -\Delta u_j &= f_j && \text{in } \Omega_j, \\ u_j &= u_{j-1} && \text{in } [a_j, b_{j-1}], \\ u_j &= u_{j+1} && \text{in } [a_{j+1}, b_j], \end{aligned} \quad (2)$$

117 where the last two conditions describe the interaction of the  $j$ -th subdomain with subdo-  
 118 mains  $j-1$  and  $j+1$ , and the function  $f_j$  is the restriction of  $f$  to  $\Omega_j$ . Notice that problem  
 119 (2) is defined for  $j = 2, \dots, N-1$ . The functions  $u_1$  and  $u_N$  of the first and the last subdo-  
 120 mains solve

$$\begin{aligned} -\Delta u_1 &= f_1 && \text{in } \Omega_1, && -\Delta u_N &= f_N && \text{in } \Omega_N, \\ u_1(a_1) &= g_1, && && u_N(b_N) &= g_N, && \\ u_1 &= u_2 && \text{in } [a_2, b_1], && u_N &= u_{N-1} && \text{in } [a_N, b_{N-1}]. \end{aligned} \quad (3)$$

Now we consider the two-dimensional model. To define each subdomain, let us consider  $L > 0$  and  $\delta > 0$ , and define the grid points  $a_j$  for  $j = 1, \dots, N+1$  and  $b_j$  for  $j = 0, \dots, N$  as shown in Figure 2. The  $j$ -th subdomain of the chain is a rectangle of dimension  $\Omega_j := (a_j, b_j) \times (0, \widehat{L})$ . Therefore, the domain of the chain is  $\Omega = \cup_{j=1}^N \Omega_j$ . As before  $2\delta$  is the overlap and  $\delta \in (0, L/2)$ . We are interested in the solution to

$$-\Delta u = f \text{ in } \Omega, \quad u = g \text{ on } \partial\Omega,$$

121 where  $f$  and  $g$  are sufficiently regular functions. We consider  $f_j$  and  $g_j$  as the restriction of  
 122  $f$  and  $g$  to the  $j$ -th subdomain. The restriction of  $u$  to  $\Omega_j$ , denoted by  $u_j$ , solves the problem

$$\begin{aligned} -\Delta u_j &= f_j && \text{in } \Omega_j, \\ u_j(\cdot, 0) &= g_j(\cdot, 0), \\ u_j(\cdot, \widehat{L}) &= g_j(\cdot, \widehat{L}), \\ u_j &= u_{j-1} && \text{in } [a_j, b_{j-1}] \times (0, \widehat{L}), \\ u_j &= u_{j+1} && \text{in } [a_{j+1}, b_j] \times (0, \widehat{L}), \end{aligned} \quad (4)$$

123 for  $j = 2, \dots, N-1$ , and

$$\begin{aligned} -\Delta u_1 &= f_1 && \text{in } \Omega_1, && -\Delta u_N &= f_N && \text{in } \Omega_N, \\ u_1(\cdot, 0) &= g_1(\cdot, 0), && && u_N(\cdot, 0) &= g_N(\cdot, 0), && \\ u_1(\cdot, \widehat{L}) &= g_1(\cdot, \widehat{L}), && && u_N(\cdot, \widehat{L}) &= g_N(\cdot, \widehat{L}), && \\ u_1(a_1, \cdot) &= g_1(a_1, \cdot), && && u_N(b_N, \cdot) &= g_N(b_N, \cdot), && \\ u_1 &= u_2 && \text{in } [a_2, b_1] \times (0, \widehat{L}), && u_N &= u_{N-1} && \text{in } [a_N, b_{N-1}] \times (0, \widehat{L}). \end{aligned} \quad (5)$$

124 The two models presented in this section seem to be very similar because of their main  
 125 one-dimensional structure (the subdomains are aligned along a straight line). However, we  
 126 will see in the following sections that they lead to completely different convergence behavior  
 127 of domain-decomposition methods.

### 128 3 Classical parallel Schwarz method

129 In this section, we study the convergence of the classical parallel Schwarz method (PSM), in  
 130 the form introduced by Lions in [31], for the problems presented in Section 2. In particular,  
 131 we analyze the behavior of the PSM for a growing number of (fixed-sized) subdomains and  
 132 investigate the corresponding weak scalability. We show that the PSM for the solution of  
 133 the one-dimensional problem (2)-(3) is not scalable, in the sense that the spectral radius  $\rho$   
 134 of the iteration matrix tends to one as  $N$  grows. On the other hand, for the two-dimensional  
 135 problem (4)-(5), we prove that there exists a function  $\bar{\rho}$ , independent of  $N$  and such that  
 136  $\rho \leq \bar{\rho} < 1$ , which means that the PSM is scalable.

#### 137 3.1 One-dimensional analysis

Consider problem (2)-(3) and an initial guess  $u_1^0, u_2^0, \dots, u_N^0$ . The PSM defines the approxi-  
 mation sequences  $\{u_j^n\}_n$  by solving

$$\begin{aligned} -\partial_{xx}u_j^n &= f_j \text{ in } (a_j, b_j), \\ u_j^n(a_j) &= u_{j-1}^{n-1}(a_j), \\ u_j^n(b_j) &= u_{j+1}^{n-1}(b_j), \end{aligned}$$

for  $j = 2, \dots, N-1$ , and

$$\begin{aligned} -\partial_{xx}u_1^n &= f_1 \text{ in } (a_1, b_1), & -\partial_{xx}u_N^n &= f_N \text{ in } (a_N, b_N), \\ u_1^n(a_1) &= 0, & u_N^n(a_N) &= u_{N-1}^{n-1}(a_N), \\ u_1^n(b_1) &= u_2^{n-1}(b_1), & u_N^n(b_N) &= 0. \end{aligned}$$

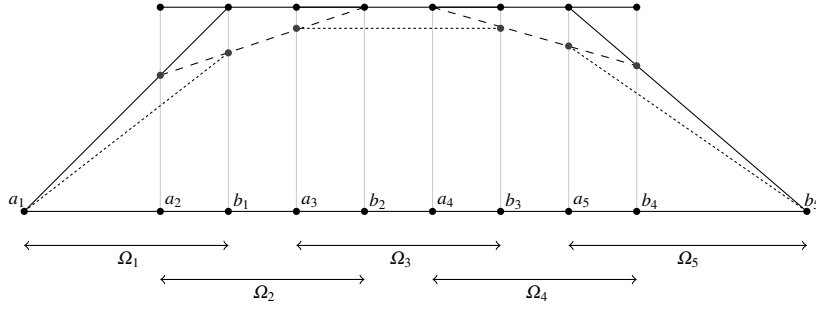
138 To analyze the convergence of this algorithm, we introduce the errors  $e_j^n := u_j - u_j^n$  and  
 139 notice that they satisfy

$$\begin{aligned} -\partial_{xx}e_j^n &= 0 \text{ in } (a_j, b_j), \\ e_j^n(a_j) &= e_{j-1}^{n-1}(a_j), \\ e_j^n(b_j) &= e_{j+1}^{n-1}(b_j), \end{aligned} \tag{6}$$

140 for  $j = 2, \dots, N-1$ , and

$$\begin{aligned} -\partial_{xx}e_1^n &= 0 \text{ in } (a_1, b_1), & -\partial_{xx}e_N^n &= 0 \text{ in } (a_N, b_N), \\ e_1^n(a_1) &= 0, & e_1^n(a_N) &= e_{N-1}^{n-1}(a_N), \\ e_1^n(b_1) &= e_2^{n-1}(b_1), & e_1^n(b_N) &= 0. \end{aligned} \tag{7}$$

141 The convergence of (6) and (7) can be established via an analysis based on the maximum  
 142 principle; see, e.g. [32, 7]. Since this analysis reveals that the PSM is not scalable, we sketch



**Fig. 3** Example of the PSM for a chain of  $N = 5$  subdomains. The solid lines are the errors at the first iteration  $e_j^1$ , the dashed lines represent  $e_j^2$ , and the dotted line is  $e_j^3$ . It is possible to observe that the contraction of the error propagates from the first and the last subdomains ( $\Omega_1$  and  $\Omega_5$ ) till the middle subdomain  $\Omega_3$ . To reach  $\Omega_3$ , the propagation needs 3 iterations.

143 it in what follows for the example in Figure 3. Let us consider an initial error  $e^0 = 1$ . The  
 144 solutions of the internal subdomains is  $e_j^1 = 1$  for  $j = 2, \dots, 4$ , whereas the solutions of the  
 145 first and the last subdomains are straight lines that have value 1 on the interface points  $b_1$   
 146 and  $a_5$  and that are zero on  $a_1$  and  $b_5$  (solid lines in Figure 3). Therefore, at the interface  
 147 points  $a_2$  and  $b_4$  the error is strictly smaller than 1, a result that holds in general for equations  
 148 that satisfy a maximum principle. This means that at the second iteration, the errors  $e_2^2$  and  
 149  $e_4^2$  (dashed lines in Figure 3) are straight lines such that  $e_2^2(a_2) = e_1^1(a_2) < 1$  and  $e_2^2(b_2) =$   
 150  $e_3^1(b_2) = 1$ , and  $e_4^2(b_4) = e_5^1(b_4) < 1$  and  $e_4^2(a_4) = e_3^1(a_4) = 1$ , whereas the errors on the  
 151 subdomains  $\Omega_1$ ,  $\Omega_3$ , and  $\Omega_5$  do not change ( $e_1^2 = e_1^1$ ,  $e_3^2 = e_3^1$ , and  $e_5^2 = e_5^1$ ). Hence, we  
 152 observe a contraction of the error in  $\Omega_2$  and  $\Omega_4$ , but the error  $e_3^2 = 1$  is still not contracting. At  
 153 the third iteration, we observe a contraction on  $\Omega_1$  and  $\Omega_5$  and, finally, also on  $\Omega_3$ , because  
 154 at the points  $a_3$  and  $b_3$  it holds that  $e_3^3(a_3) = e_2^2(a_3) < 1$  and  $e_3^3(b_3) = e_4^2(b_3) < 1$ , which  
 155 implies by the maximum principle that  $e_3^3(x) < 1$  (dotted lines in Figure 3). This example  
 156 shows that, to observe a contraction in the subdomain in the middle of the chain, that is  $\Omega_3$ ,  
 157 we have to wait 3 iterations. By induction, we thus have to wait about  $N/2$  iterations before  
 158 observing a contraction of the error in the subdomains in the middle of the chain. Hence,  
 159 for a growing number of subdomains  $N$  one has to wait more and more iterations before the  
 160 error contracts on each subdomain in the chain. This observation indicates that the PSM for  
 161 the solution of the one-dimensional problem (2)-(3) is not scalable.

We study now in detail the convergence of the PSM (6)-(7), whose solutions are

$$e_j^n(x) = e_{j-1}^{n-1}(a_j) + \frac{x-a_j}{b_j-a_j} (e_{j+1}^{n-1}(b_j) - e_{j-1}^{n-1}(a_j)),$$

for  $j = 2, \dots, N-1$ , and

$$e_1^n(x) = \frac{x-a_1}{b_1-a_1} e_2^{n-1}(b_1), \quad e_N^n(x) = \left(1 - \frac{x-a_N}{b_N-a_N}\right) e_{N-1}^{n-1}(a_N).$$

Evaluating  $e_j^n$  at the interface points and defining the vector

$$\mathbf{e}^n := [0, e_2^n(b_1), e_1^n(a_2), e_3^n(b_2), \dots, e_{j-1}^n(a_j), e_{j+1}^n(b_j), \dots, e_{N-2}^n(a_{N-1}), e_N^n(b_{N-1}), e_{N-1}^n(a_N), 0]^\top,$$

we get

$$\mathbf{e}^n = T_{1D} \mathbf{e}^{n-1},$$



## 164 3.2 Two-dimensional analysis

In this section, we study the PSM for the solution to (4)-(5). The analysis we present is mainly based on the results obtained in [6], but we consider a different construction of the iteration matrix, which is similar to the one considered for the other methods in the following sections. The PSM is given by

$$\begin{aligned} -\Delta u_j^n &= f_j \text{ in } \Omega_j, \\ u_j^n(\cdot, 0) &= g_j(\cdot, 0), \\ u_j^n(\cdot, \widehat{L}) &= g_j(\cdot, \widehat{L}), \\ u_j^n(a_j, \cdot) &= u_{j-1}^{n-1}(a_j, \cdot), \\ u_j^n(b_j, \cdot) &= u_{j+1}^{n-1}(b_j, \cdot), \end{aligned}$$

for  $j = 2, \dots, N-1$ , and

$$\begin{aligned} -\Delta u_1^n &= f_1 \text{ in } \Omega_1, & -\Delta u_N^n &= f_N \text{ in } \Omega_N, \\ u_1^n(\cdot, 0) &= g_1(\cdot, 0), & u_N^n(\cdot, 0) &= g_N(\cdot, 0), \\ u_1^n(\cdot, \widehat{L}) &= g_1(\cdot, \widehat{L}), & u_N^n(\cdot, \widehat{L}) &= g_N(\cdot, \widehat{L}), \\ u_1^n(a_1, \cdot) &= g_1(a_1, \cdot), & u_N^n(a_N, \cdot) &= u_{N-1}^{n-1}(a_N, \cdot), \\ u_1^n(b_1, \cdot) &= u_2^{n-1}(b_1, \cdot), & u_N^n(b_N, \cdot) &= g_N(b_N, \cdot). \end{aligned}$$

165 Introducing again the errors  $e_j^n := u_j - u_j^n$ , the PSM becomes

$$\begin{aligned} -\Delta e_j^n &= 0 \text{ in } \Omega_j, \\ e_j^n(\cdot, 0) &= 0, \quad e_j^n(\cdot, \widehat{L}) = 0, \\ e_j^n(a_j, \cdot) &= e_{j-1}^{n-1}(a_j, \cdot), \\ e_j^n(b_j, \cdot) &= e_{j+1}^{n-1}(b_j, \cdot), \end{aligned} \tag{9}$$

166 for  $j = 2, \dots, N-1$ , and

$$\begin{aligned} -\Delta e_1^n &= 0 \text{ in } \Omega_1, & -\Delta e_N^n &= 0 \text{ in } \Omega_N, \\ e_1^n(\cdot, 0) &= 0, \quad e_1^n(\cdot, \widehat{L}) = 0, & e_N^n(\cdot, 0) &= 0, \quad e_N^n(\cdot, \widehat{L}) = 0, \\ e_1^n(a_1, \cdot) &= 0, & e_N^n(a_N, \cdot) &= e_{N-1}^{n-1}(a_N, \cdot), \\ e_1^n(b_1, \cdot) &= e_2^{n-1}(b_1, \cdot), & e_N^n(b_N, \cdot) &= 0. \end{aligned} \tag{10}$$

To construct the Schwarz iteration matrix corresponding to (9)-(10), we use the Fourier sine expansion

$$e_j^n(x, y) = \sum_{m=1}^{\infty} v_j^n(x, k) \sin(ky), \quad k = \frac{\pi m}{\widehat{L}},$$

where the Fourier coefficients  $v_j^n(x, k)$  are given by

$$v_j^n(x, k) = \widetilde{c}_j(k, \delta) e^{kx} + \widetilde{d}_j(k, \delta) e^{-kx},$$

167 and  $\widetilde{c}_j(k, \delta)$  and  $\widetilde{d}_j(k, \delta)$  are computed using the conditions  $v_j^n(a_j, k) = v_{j-1}^{n-1}(a_j, k)$  and

168  $v_j^n(b_j, k) = v_{j+1}^{n-1}(b_j, k)$ , which are obtained by using the transmission conditions. Notice



169 that  $k$  is parametrized by  $m$ , hence one should formally write  $k_m$ , but we drop the subscript  
170  $m$  for simplicity. For  $j = 2, \dots, N-1$ , we obtain that

$$\begin{aligned} v_j^n(x, k) &= e^{kx} e^{-jkL} \left[ g_{A1}(k, \delta) v_{j+1}^{n-1}(b_j, k) - g_{A2}(k, \delta) v_{j-1}^{n-1}(a_j, k) \right] \\ &\quad + e^{-kx} e^{jkL} \left[ g_{B1}(k, \delta) v_{j-1}^{n-1}(a_j, k) - g_{B2}(k, \delta) v_{j+1}^{n-1}(b_j, k) \right] \end{aligned} \quad (11)$$

with

$$\begin{aligned} g_{A1}(k, \delta) &:= \frac{e^{3k\delta+2kL}}{e^{4k\delta+2kL} - 1}, & g_{A2}(k, \delta) &:= \frac{e^{k\delta+kL}}{e^{4k\delta+2kL} - 1}, \\ g_{B1}(k, \delta) &:= \frac{e^{3k\delta+kL}}{e^{4k\delta+2kL} - 1}, & g_{B2}(k, \delta) &:= \frac{e^{k\delta}}{e^{4k\delta+2kL} - 1}. \end{aligned}$$

171 We rewrite (11) in the form

$$v_j^n(x, k) = w_j(x, k; \delta) v_{j+1}^{n-1}(b_j, k) + z_j(x, k; \delta) v_{j-1}^{n-1}(a_j, k), \quad (12)$$

where

$$\begin{aligned} w_j(x, k; \delta) &:= e^{kx} e^{-jkL} g_{A1}(k, \delta) - e^{-kx} e^{jkL} g_{B2}(k, \delta), \\ z_j(x, k; \delta) &:= e^{-kx} e^{jkL} g_{B1}(k, \delta) - e^{kx} e^{-jkL} g_{A2}(k, \delta). \end{aligned}$$

In a similar fashion, solving problems (10), we get

$$v_1^n(x, k) = w_1(x, k; \delta) v_2^{n-1}(b_1, k), \quad v_N^n(x, k) = z_N(x, k; \delta) v_{N-1}^{n-1}(a_N, k),$$

with

$$\begin{aligned} w_1(x, k; \delta) &:= \frac{e^{k\delta+kL}}{1 - e^{4k\delta+2kL}} \left[ e^{-kx} - e^{2k\delta+kx} \right], \\ z_N(x, k; \delta) &:= \frac{e^{k\delta+kL}}{1 - e^{4k\delta+2kL}} \left[ e^{kx-kNL} - e^{kNL+2k\delta-kx} \right]. \end{aligned}$$

172 Now, we define

$$\begin{aligned} w_a(k, \delta) &:= w_j(a_{j+1}, k; \delta) = w_{j-1}(a_j, k; \delta), \\ w_b(k, \delta) &:= w_{j+1}(b_j, k; \delta) = w_j(b_{j-1}, k; \delta), \\ z_a(k, \delta) &:= z_j(a_{j+1}, k; \delta) = z_{j-1}(a_j, k; \delta), \\ z_b(k, \delta) &:= z_{j+1}(b_j, k; \delta) = z_j(b_{j-1}, k; \delta), \end{aligned} \quad (13)$$

173 and a direct calculation [6] shows that  $z_b(k, \delta) = \frac{e^{2k\delta+2kL} - e^{2k\delta}}{e^{4k\delta+2kL} - 1}$ ,  $w_b(k, \delta) = \frac{e^{4k\delta+kL} - e^{kL}}{e^{4k\delta+2kL} - 1}$ , with

$$(z_b + w_b)(k, \delta) = \frac{e^{2k\delta} + e^{kL}}{e^{2k\delta+kL} + 1}. \quad (14)$$

174 We recall the following results [6, Lemma 1 and Lemma 2].

175 **Lemma 1** For any  $(k, \delta) \in (0, \infty) \times [0, L]$ , the quantities defined in (13) satisfy  $w_a(k, \delta) \geq 0$   
176 and  $w_b(k, \delta) \geq 0$ . Moreover  $w_a(k, \delta) = z_b(k, \delta)$  and  $w_b(k, \delta) = z_a(k, \delta)$ .

177 **Lemma 2** The following statements hold:



190 Theorem 1 shows that the PSM for the solution of the two-dimensional problem con-  
 191 verges and the spectral radius (its contraction factor) does not deteriorate as  $N$  grows, be-  
 192 cause  $\rho(T_{2D}(k, \delta)) \leq \|T_{2D}(k, \delta)\|_\infty \leq \bar{\rho}(\delta) < 1$  for any  $N$ . This means that the PSM for the  
 193 solution of the two-dimensional problem is weakly scalable. In Figure 4 (right) the spectral  
 194 radius  $\rho(T_{2D})$  (blue line) and the norm  $\|T_{2D}\|_\infty$  (red line) are shown as a function of  $N$ : as  $N$   
 195 increases, the spectral radius grows, but it is bounded by the infinity-norm which is strictly  
 196 smaller than one.

#### 197 4 Optimized Schwarz method

198 The classical Schwarz method, despite its flexibility and generality, has major drawbacks  
 199 such as the requirement of overlap, lack of convergence for some PDEs and slow conver-  
 200 gence speed in general [14]. In the pioneering paper [33], Lions proposed to exploit (general-  
 201 ized) Robin conditions as transmission conditions on the interfaces between subdomains  
 202 to obtain a convergent Schwarz method without overlap. To improve the convergence be-  
 203 havior, one can optimize the Robin parameter, as it was shown in [28]. The generalization  
 204 of this idea led to overlapping and non-overlapping optimized Schwarz methods (OSMs),  
 205 which have extensively been studied over the last decades, see [13] for a review, [22] for  
 206 Helmholtz problems, [9] for Maxwell equations and [26] for advection diffusion equations.  
 207 More recent applications to heterogeneous problems can be found in [15, 25].

208 We investigate now the scalability of the OSM for the one- and two-dimensional model  
 209 problems introduced in Section 2. Like for the classical parallel Schwarz method, we show  
 210 that the OSM is scalable for the solution of the two-dimensional problem, but not for the  
 211 one-dimensional one, and we will also give some insight on the optimal choice for the Robin  
 212 parameter.

##### 213 4.1 Optimized Schwarz method in 1D

214 The error equations associated to the OSM for (2)-(3) are given by

$$\begin{aligned} \partial_{xx}e_j^n &= 0 \text{ in } (a_j, b_j), \\ \partial_x e_j^n(a_j) - p e_j^n(a_j) &= \partial_x e_{j-1}^{n-1}(a_j) - p e_{j-1}^{n-1}(a_j), \\ \partial_x e_j^n(b_j) + p e_j^n(b_j) &= \partial_x e_{j+1}^{n-1}(b_j) + p e_{j+1}^{n-1}(b_j), \end{aligned} \quad (15)$$

215 for  $j = 2, \dots, N-1$ , where  $p$  is the Robin parameter, and

$$\begin{aligned} \partial_{xx}e_1^n &= 0 \text{ in } (a_1, b_1), \\ e_1^n(a_1) &= 0, \\ \partial_x e_1^n(b_1) + p e_1^n(b_1) &= \partial_x e_2^{n-1}(b_1) + p e_2^{n-1}(b_1), \end{aligned} \quad (16)$$

216 and

$$\begin{aligned} \partial_{xx}e_N^n &= 0 \text{ in } (a_N, b_N), \\ \partial_x e_N^n(a_N) - p e_N^n(a_N) &= \partial_x e_{N-1}^{n-1}(a_N) - p e_{N-1}^{n-1}(a_N), \\ e_N^n(b_N) &= 0. \end{aligned} \quad (17)$$

217 The corresponding solution in  $\Omega_j$  is given by

$$e_j^n(x) = A_j^n x + B_j^n. \quad (18)$$

218 Defining

$$\begin{aligned} \mathcal{R}_-^{n-1}(a_j) &:= \partial_x e_{j-1}^{n-1}(a_j) - p e_{j-1}^{n-1}(a_j), \\ \mathcal{R}_+^{n-1}(b_j) &:= \partial_x e_{j+1}^{n-1}(b_j) + p e_{j+1}^{n-1}(b_j), \end{aligned} \quad (19)$$

and inserting (18) into the boundary conditions in (15), we get the linear system

$$\begin{aligned} A_j^n - p A_j^n a_j - p B_j^n &= \mathcal{R}_-^{n-1}(a_j), \\ A_j^n + p A_j^n b_j + p B_j^n &= \mathcal{R}_+^{n-1}(b_j), \end{aligned}$$

whose solution is

$$A_j^n = \frac{1}{\kappa} p (\mathcal{R}_-^{n-1}(a_j) + \mathcal{R}_+^{n-1}(b_j)), \quad B_j^n = \frac{1}{\kappa} ((1 - p a_j) \mathcal{R}_+^{n-1}(b_j) - (1 + p b_j) \mathcal{R}_-^{n-1}(a_j)),$$

219 with  $\kappa := 2p + p^2(L + 2\delta)$ . Inserting  $A_j^n$  and  $B_j^n$  into (18) and using  $b_j = a_j + L + 2\delta$ , we get

$$\begin{aligned} e_j^n(x) &= \frac{1}{\kappa} \left[ p (\mathcal{R}_-^{n-1}(a_j) + \mathcal{R}_+^{n-1}(b_j)) x + \mathcal{R}_+^{n-1}(b_j) - \mathcal{R}_-^{n-1}(a_j) \right. \\ &\quad \left. - p a_j (\mathcal{R}_-^{n-1}(a_j) + \mathcal{R}_+^{n-1}(b_j)) - p(L + 2\delta) \mathcal{R}_-^{n-1}(a_j) \right]. \end{aligned} \quad (20)$$

Now, we construct the iteration matrix of the OSM. To do so, we recall the definition (19) of  $\mathcal{R}_-^{n-1}(a_j)$  and  $\mathcal{R}_+^{n-1}(b_j)$  and insert (20) in to (19) to obtain, for  $j = 2, \dots, N-1$ , that

$$\begin{bmatrix} \mathcal{R}_-^n(a_j) \\ \mathcal{R}_+^n(b_j) \end{bmatrix} = T_1 \begin{bmatrix} \mathcal{R}_-^{n-1}(a_{j-1}) \\ \mathcal{R}_+^{n-1}(b_{j-1}) \end{bmatrix} + T_2 \begin{bmatrix} \mathcal{R}_-^{n-1}(a_{j+1}) \\ \mathcal{R}_+^{n-1}(b_{j+1}) \end{bmatrix},$$

where

$$T_1 := \frac{p}{\kappa} \begin{bmatrix} (2 - pL + p(L + 2\delta)) & -pL \\ 0 & 0 \end{bmatrix}, \quad T_2 := \frac{p}{\kappa} \begin{bmatrix} 0 & 0 \\ 2p\delta - p(L + 2\delta) & (2 + 2p\delta) \end{bmatrix}.$$

Similarly, for the subdomains  $\Omega_1, \Omega_2, \Omega_{N-1}$ , and  $\Omega_N$  we obtain

$$\begin{aligned} \begin{bmatrix} 0 \\ \mathcal{R}_+^n(b_1) \end{bmatrix} &= T_2 \begin{bmatrix} \mathcal{R}_-^{n-1}(a_2) \\ \mathcal{R}_+^{n-1}(b_2) \end{bmatrix}, \\ \begin{bmatrix} \mathcal{R}_-^n(a_2) \\ \mathcal{R}_+^n(b_2) \end{bmatrix} &= \tilde{T}_1 \begin{bmatrix} 0 \\ \mathcal{R}_+^{n-1}(b_1) \end{bmatrix} + T_2 \begin{bmatrix} \mathcal{R}_-^{n-1}(a_3) \\ \mathcal{R}_+^{n-1}(b_3) \end{bmatrix}, \\ \begin{bmatrix} \mathcal{R}_-^n(a_{N-1}) \\ \mathcal{R}_+^n(b_{N-1}) \end{bmatrix} &= T_1 \begin{bmatrix} \mathcal{R}_-^{n-1}(a_{N-2}) \\ \mathcal{R}_+^{n-1}(b_{N-2}) \end{bmatrix} + \tilde{T}_2 \begin{bmatrix} \mathcal{R}_-^{n-1}(a_n) \\ 0 \end{bmatrix}, \\ \begin{bmatrix} \mathcal{R}_-^n(a_N) \\ 0 \end{bmatrix} &= T_1 \begin{bmatrix} \mathcal{R}_-^{n-1}(a_{N-1}) \\ \mathcal{R}_+^{n-1}(b_{N-1}) \end{bmatrix}, \end{aligned}$$

where

$$\tilde{T}_1 := \begin{bmatrix} 0 & \frac{1-pL}{(1+p(L+2\delta))} \\ 0 & 0 \end{bmatrix}, \quad \tilde{T}_2 := \begin{bmatrix} 0 & 0 \\ \frac{1-pL}{(1+p(L+2\delta))} & 0 \end{bmatrix}.$$



228 We now show that it is possible to make the one-dimensional OSM convergent in a  
 229 finite number of iterations. To do so, we use a different Robin parameter  $p$  in (15) for each  
 230 subdomain  $\Omega_j$ , namely

$$\begin{aligned} \partial_{xx}e_j^n &= 0 \text{ in } (a_j, b_j), \\ \partial_x e_j^n(a_j) - p_j^- e_j^n(a_j) &= \partial_x e_{j-1}^{n-1}(a_j) - p_j^- e_{j-1}^{n-1}(a_j), \\ \partial_x e_j^n(b_j) + p_j^+ e_j^n(b_j) &= \partial_x e_{j+1}^{n-1}(b_j) + p_j^+ e_{j+1}^{n-1}(b_j), \end{aligned} \quad (23)$$

231 where  $p_j^- > 0$  and  $p_j^+ > 0$  are given by the following theorem, which is proved using similar  
 232 arguments as in [5].

233 **Theorem 2** Let  $L_j^+ := b_N - b_j, j = 1, \dots, N-1, L_j^- := a_j - a_1, j = 2, \dots, N$ . If we set  $p_j^+ :=$   
 234  $1/L_j^+, j = 1, \dots, N-1, p_j^- = 1/L_{j-1}^-, j = 2, \dots, N$ , then the OSM (23) converges exactly in  
 235  $N$  iterations.

*Proof* First we prove that  $p_j^+, p_j^-$ , satisfy the following property:

$$\partial_x e_j^n + p_j^+ e_j^n = 0 \text{ on } x = b_j \quad \implies \quad \partial_x e_j^n + p_{j-1}^+ e_j^n = 0 \text{ on } x = b_{j-1}, \quad (24)$$

$$\partial_x e_j^n - p_j^- e_j^n = 0 \text{ on } x = a_{j-1} \quad \implies \quad \partial_x e_j^n - p_{j+1}^- e_j^n = 0 \text{ on } x = a_j. \quad (25)$$

236 To do so, suppose that  $\partial_x e_j^n(b_j) + p_j^+ e_j^n(b_j) = 0$ . Let  $v$  be defined on  $(b_{j-1}, b_N)$  by  $v(x) :=$   
 237  $\frac{e_j^n(b_{j-1})}{L_{j-1}^+}(b_N - x)$ , we have that  $\partial_x v(b_j) + p_j^+ v(b_j) = 0$  and by construction  $v(b_{j-1}) = e_j^n(b_{j-1})$ .

238 Hence  $v$  satisfies

$$\begin{aligned} -\partial_{xx}(e_j^n - v) &= 0 \text{ in } (b_{j-1}, b_j), \\ e_j^n - v &= 0 \text{ on } x = b_{j-1}, \\ (\partial_x + p_j^+)(e_j^n - v) &= 0 \text{ on } x = b_j. \end{aligned} \quad (26)$$

By uniqueness of the solution of (26) we have that  $e_j^n = v$  on  $(b_{j-1}, b_j)$ , and we conclude that  
 $\partial_x e_j^n(b_{j-1}) + p_{j-1}^+ e_j^n(b_{j-1}) = 0$  since this holds for  $v$ . Similarly, suppose that  $\partial_x e_j^n(a_{j-1}) -$   
 $p_j^- e_j^n(a_{j-1}) = 0$ , and let  $w$  be defined on  $(a_0, a_j)$  by  $w(x) = \frac{e_j^n(x_j)}{L_j^-}(x - a_0)$ . It holds that  
 $\partial_x w(a_{j-1}) - p_j^- w(a_{j-1}) = 0$  and  $w(a_j) = e_j^n(a_j)$ . Hence  $w$  verifies

$$\begin{aligned} \partial_{xx}(e_j^n - w) &= 0 \text{ in } (a_{j-1}, a_j), \\ (\partial_x - p_j^-)(e_j^n - w) &= 0 \text{ on } x = a_{j-1}, \\ e_j^n - w &= 0 \text{ on } x = a_j, \end{aligned}$$

239 which implies that  $e_j^n = w$ . Therefore  $\partial_x e_j^n(a_j) - p_{j+1}^- e_j^n(a_j) = 0$ .

Now we prove that the OSM (23) converges in  $N$  iterations. A direct calculation shows  
 that the choices  $p_2^- = \frac{1}{L_1^-}$  and  $p_{N-1}^+ = \frac{1}{L_{N-1}^+}$  imply that  $\partial_x e_1^n(a_1) - p_2^- e_1^n(a_1) = 0$  and  $\partial_x e_N^n(b_{N-1}) +$   
 $p_{N-1}^+ e_N^n(b_{N-1}) = 0$  for any  $n \geq 0$ . Hence, the transmission conditions in (23) allow us to  
 write

$$\begin{aligned} \partial_x e_2^{n+1}(a_1) - p_2^- e_2^{n+1}(a_1) &= \partial_x e_1^n(a_1) - p_2^- e_1^n(a_1) = 0, \\ \partial_x e_{N-1}^{n+1}(b_{N-1}) + p_{N-1}^+ e_{N-1}^{n+1}(b_{N-1}) &= \partial_x e_N^n(b_{N-1}) + p_{N-1}^+ e_N^n(b_{N-1}) = 0, \end{aligned}$$

for any  $n \geq 0$ . Using (24) and (25) and again the transmission conditions in (23), we get

$$\begin{aligned} \partial_x e_3^{n+1}(a_2) - p_3^- e_3^{n+1}(a_2) &= \partial_x e_2^n(a_2) - p_3^- e_2^n(a_2) = 0, \\ \partial_x e_{N-2}^{n+1}(b_{N-2}) + p_{N-2}^+ e_{N-2}^{n+1}(b_{N-2}) &= \partial_x e_{N-1}^n(b_{N-2}) + p_{N-2}^+ e_{N-1}^n(b_{N-2}) = 0, \end{aligned}$$

for  $n \geq 1$ . By induction, we obtain that after  $N$  iterations that the errors  $e_j^N$  satisfy

$$\begin{aligned} -\partial_{xx} e_j^N &= 0 \text{ in } (a_j, b_j), \\ (\partial_x + p_j^+) e_j^N &= 0 \text{ on } x = b_j, \\ (\partial_x - p_j^-) e_j^N &= 0 \text{ on } x = a_j, \end{aligned}$$

and

$$\begin{aligned} -\partial_{xx} e_1^N &= 0 \text{ in } (a_1, b_1), & -\partial_{xx} e_N^N &= 0 \text{ in } (a_N, b_N), \\ e_1^N &= 0 \text{ on } x = a_1, & (\partial_x - p_N^-) e_N^N &= 0 \text{ on } x = a_N, \\ (\partial_x + p_1^+) e_1^N &= 0 \text{ on } x = b_1, & e_N^N &= 0 \text{ on } x = b_N. \end{aligned}$$

240 Hence  $e_j^N = 0$ , for  $j = 1 \dots, N$ , which concludes our proof.

241 The one-dimensional result above can be generalized to higher dimensions by replacing  
242 the parameter  $p$  with a suitably chosen global operator (in general a Dirichlet-to-Neumann  
243 operator), see [36]. This choice is computationally expensive in practice, and hence the  
244 global operator is often approximated by local operators [28].

#### 245 4.2 Optimized Schwarz method in 2D

246 Let us consider problem (4)-(5). The OSM (in error form) is given by

$$\begin{aligned} -\Delta e_j^n &= 0 \text{ in } \Omega_j, \\ e_j^n(\cdot, 0) &= 0, \quad e_j^n(\cdot, \widehat{L}) = 0, \\ \partial_x e_j^n(a_j, \cdot) - p e_j^n(a_j, \cdot) &= \partial_x e_{j-1}^{n-1}(a_j, \cdot) - p e_{j-1}^{n-1}(a_j, \cdot), \\ \partial_x e_j^n(b_j, \cdot) + p e_j^n(b_j, \cdot) &= \partial_x e_{j+1}^{n-1}(b_j, \cdot) + p e_{j+1}^{n-1}(b_j, \cdot), \end{aligned} \quad (27)$$

for  $j = 2, \dots, N-1$ , and

$$\begin{aligned} -\Delta e_1^n &= 0 \text{ in } \Omega_1, & -\Delta e_N^n &= 0 \text{ in } \Omega_N, \\ e_1^n(\cdot, 0) &= 0, \quad e_1^n(\cdot, \widehat{L}) = 0, & e_N^n(\cdot, 0) &= 0, \quad e_N^n(\cdot, \widehat{L}) = 0, \\ e_1^n(a_1, \cdot) &= 0, & (\partial_x - p) e_N^n(a_N, \cdot) &= (\partial_x - p) e_{N-1}^{n-1}(a_N, \cdot), \\ (\partial_x + p) e_1^n(b_1, \cdot) &= (\partial_x + p) e_2^{n-1}(b_1, \cdot), & e_N^n(b_N, \cdot) &= 0. \end{aligned}$$

247 As in Section 3.2, we use the Fourier expansion  $e_j^n(x, y) = \sum_{m=1}^{\infty} v_j^n(x, k) \sin(ky)$  with  $k = \frac{\pi m}{L}$ .  
248 The Fourier coefficients  $v_j^n$  must satisfy

$$\begin{aligned} \partial_{xx} v_j^n &= k^2 v_j^n \text{ in } (a_j, b_j), \\ \partial_x v_j^n(a_j) - p v_j^n(a_j) &= \partial_x v_{j-1}^{n-1}(a_j) - p v_{j-1}^{n-1}(a_j), \\ \partial_x v_j^n(b_j) + p v_j^n(b_j) &= \partial_x v_{j+1}^{n-1}(b_j) + p v_{j+1}^{n-1}(b_j). \end{aligned} \quad (28)$$

249 Defining  $\mathcal{R}_-^{n-1}(a_j) := \partial_x v_{j-1}^{n-1}(a_j) - p v_{j-1}^{n-1}(a_j)$  and  $\mathcal{R}_+^{n-1}(b_j) := \partial_x v_{j+1}^{n-1}(b_j) + p v_{j+1}^{n-1}(b_j)$ ,  
 250 the solution to (28) is given by

$$\begin{aligned} v_j^n(x, k) = & \mathcal{R}_-^{n-1}(a_j) \left[ -\frac{1}{\gamma}(k-p)e^{k(x-b_j)} - \frac{1}{\gamma}(k+p)e^{k(b_j-x)} \right] \\ & + \mathcal{R}_+^{n-1}(b_j) \left[ \frac{1}{\gamma}(k+p)e^{k(x-a_j)} + \frac{1}{\gamma}(k-p)e^{k(a_j-x)} \right], \end{aligned} \quad (29)$$

251 where  $\gamma := (k+p)^2 e^{k(L+2\delta)} - (k-p)^2 e^{-k(L+2\delta)}$ . As for the 1D case, we insert (29) into the  
 252 definitions of  $\mathcal{R}_-^n(a_j)$  and  $\mathcal{R}_+^n(b_j)$  to get

$$\begin{bmatrix} \mathcal{R}_-^n(a_j) \\ \mathcal{R}_+^n(b_j) \end{bmatrix} = T_1 \begin{bmatrix} \mathcal{R}_-^{n-1}(a_{j-1}) \\ \mathcal{R}_+^{n-1}(b_{j-1}) \end{bmatrix} + T_2 \begin{bmatrix} \mathcal{R}_-^{n-1}(a_{j+1}) \\ \mathcal{R}_+^{n-1}(b_{j+1}) \end{bmatrix}, \quad (30)$$

where

$$T_1 := \begin{bmatrix} g_3 - pg_1 & g_4 - pg_2 \\ 0 & 0 \end{bmatrix}, \quad T_2 := \begin{bmatrix} 0 & 0 \\ g_4 - pg_2 & g_3 - pg_1 \end{bmatrix},$$

253 with

$$\begin{aligned} g_1 &:= -\frac{1}{\gamma}(k-p)e^{-2\delta k} - \frac{1}{\gamma}(k+p)e^{2\delta k}, & g_2 &:= \frac{1}{\gamma}(k+p)e^{kL} + \frac{1}{\gamma}(k-p)e^{-kL}, \\ g_3 &:= \frac{-k}{\gamma}(k-p)e^{-2\delta k} + \frac{k}{\gamma}(k+p)e^{2\delta k}, & g_4 &:= \frac{k}{\gamma}(k+p)e^{kL} - \frac{k}{\gamma}(k-p)e^{-kL}. \end{aligned} \quad (31)$$

254 Similar arguments allow us to obtain for the subdomains  $\Omega_1, \Omega_2, \Omega_{N-1}$ , and  $\Omega_N$  the relations

$$\begin{aligned} \begin{bmatrix} 0 \\ \mathcal{R}_+^n(b_1) \end{bmatrix} &= T_2 \begin{bmatrix} \mathcal{R}_-^{n-1}(a_2) \\ \mathcal{R}_+^{n-1}(b_2) \end{bmatrix}, \\ \begin{bmatrix} \mathcal{R}_-^n(a_2) \\ \mathcal{R}_+^n(b_2) \end{bmatrix} &= \tilde{T}_1 \begin{bmatrix} 0 \\ \mathcal{R}_+^{n-1}(b_1) \end{bmatrix} + T_2 \begin{bmatrix} \mathcal{R}_-^{n-1}(a_3) \\ \mathcal{R}_+^{n-1}(b_3) \end{bmatrix}, \\ \begin{bmatrix} \mathcal{R}_-^n(a_{N-1}) \\ \mathcal{R}_+^n(b_{N-1}) \end{bmatrix} &= T_1 \begin{bmatrix} \mathcal{R}_-^{n-1}(a_{N-2}) \\ \mathcal{R}_+^{n-1}(b_{N-2}) \end{bmatrix} + \tilde{T}_2 \begin{bmatrix} \mathcal{R}_-^{n-1}(a_N) \\ 0 \end{bmatrix}, \\ \begin{bmatrix} \mathcal{R}_-^n(a_N) \\ 0 \end{bmatrix} &= T_1 \begin{bmatrix} \mathcal{R}_-^{n-1}(a_{N-1}) \\ \mathcal{R}_+^{n-1}(b_{N-1}) \end{bmatrix}, \end{aligned} \quad (32)$$

where

$$\tilde{T}_1 := \begin{bmatrix} 0 & \frac{(k+p)e^{-kL} + (k-p)e^{kL}}{(k+p)e^{k(L+2\delta)} + (k-p)e^{-k(L+2\delta)}} \\ 0 & 0 \end{bmatrix}, \quad \tilde{T}_2 := \begin{bmatrix} 0 & 0 \\ \frac{(k+p)e^{-kL} + (k-p)e^{kL}}{(k+p)e^{k(L+2\delta)} + (k-p)e^{-k(L+2\delta)}} & 0 \end{bmatrix}.$$

255 Similarly as in Section 4.1 we use (30)-(32) to construct the iteration relation  $\mathbf{r}^n = T_{2D}^O \mathbf{r}^{n-1}$ ,  
 256 where  $T_{2D}^O$  is a block matrix with the same structure as in (22). We are now ready to prove  
 257 scalability of the OSM in the overlapping case:

258 **Theorem 3** Recall (31) and define  $\varphi(k, \delta, p) := |g_3 - pg_1| + |g_4 - pg_2|$ . The OSM with over-  
 259 lap,  $\delta > 0$ , for the solution of problem (27) is scalable, in the sense that  $\rho(T_{2D}^O(k, \delta, p)) \leq$   
 260  $\|T_{2D}^O(k, \delta, p)\|_\infty \leq \max_k \max\{\varphi(k, \delta, p), \|\tilde{T}_1(k, \delta, p)\|_\infty\} < 1$  (independently of  $N$ ) for every  
 261  $p \geq 0$ .



*Proof* Because of the structure of  $T_{2D}^O$  (as in (22)), the norm  $\|T_{2D}^O\|_\infty$  is given by

$$\|T_{2D}^O\|_\infty = \max_i \sum_j |(T_{2D}^O)_{i,j}| = \max\{\varphi(k, \delta, p), \|\tilde{T}_1\|_\infty, \|\tilde{T}_2\|_\infty\}.$$

We begin by showing that  $\varphi(k, \delta, p) < 1$  for any  $k, p \in [0, \infty)$  and  $\delta > 0$ . To do so, we notice that

$$\begin{aligned} |g_3 - pg_1| &= \left| \frac{1}{\gamma} (-k(k-p)e^{-2\delta k} + k(k+p)e^{2\delta k} + p(k-p)e^{-2\delta k} + p(k+p)e^{2\delta k}) \right| \\ &= \frac{1}{\gamma} |(k+p)^2 e^{2\delta k} - (k-p)^2 e^{-2\delta k}| = \frac{1}{\gamma} ((k+p)^2 e^{2\delta k} - (k-p)^2 e^{-2\delta k}) \end{aligned}$$

and

$$\begin{aligned} |g_4 - pg_2| &= \frac{1}{\gamma} |(k(k-p)e^{kL} - k(k-p)e^{-kL} - p(k+p)e^{kL} - p(k-p)e^{-kL})| \\ &= \frac{1}{\gamma} (k+p)|k-p|(e^{kL} - e^{-kL}), \end{aligned}$$

which implies that

$$\varphi(k, \delta, p) = \frac{(k+p)^2 e^{2\delta k} - (k-p)^2 e^{-2\delta k} + (k+p)|k-p|(e^{kL} - e^{-kL})}{(k+p)^2 e^{kL+2k\delta} - (k-p)^2 e^{-kL-2k\delta}}.$$

By computing the derivative of  $\varphi$  with respect to  $p$  we find

$$\begin{aligned} \frac{\partial \varphi}{\partial p} &= - \frac{2ke^{2\delta k+2kL} - 2ke^{2\delta k}}{k^2 e^{4\delta k} + 2ke^{4\delta k} + p^2 e^{4\delta k} e^{2kL} + 2k^2 e^{2\delta k} - 2e^{2\delta k} p^2 e^{kL} + (p-k)^2} \quad \text{for } p < k, \\ \frac{\partial \varphi}{\partial p} &= \frac{2ke^{2\delta k+2kL} - 2ke^{2\delta k}}{k^2 e^{4\delta k} + 2ke^{4\delta k} + p^2 e^{4\delta k} e^{2kL} + 2p^2 e^{2\delta k} - 2e^{2\delta k} k^2 e^{kL} + (k-p)^2} \quad \text{for } p > k. \end{aligned}$$

Analyzing the signs of these derivatives, we see that  $\varphi(k, \delta, p)$  is strictly decreasing for  $p < k$  and it is strictly increasing for  $p > k$ , thus it reaches a minimum for  $p = k$ . Therefore the maximum of  $\varphi(k, \delta, p)$  with respect to the variable  $p$  is obtained for  $p = 0$  and for  $p \rightarrow +\infty$ :

$$\varphi(k, \delta, p) \leq \max\{\varphi(k, \delta, 0), \lim_{p \rightarrow \infty} \varphi(k, \delta, p)\}.$$

For  $p = 0$ ,  $\delta > 0$  and  $L > 0$  we have

$$\begin{aligned} \varphi(k, \delta, p) &= \frac{e^{2\delta k} - e^{-2\delta k} + e^{kL} - e^{-kL}}{e^{kL+2\delta k} - e^{-kL-2\delta k}} \\ &= \frac{\sinh(2\delta k) + \sinh(kL)}{\sinh(kL) \cosh(2\delta k) + \sinh(2\delta k) \cosh(kL)} < 1, \end{aligned}$$

and, under the same conditions,

$$\lim_{p \rightarrow \infty} \varphi(k, \delta, p) = \frac{\sinh(2\delta k) + \sinh(kL)}{\sinh(kL) \cosh(2\delta k) + \sinh(2\delta k) \cosh(kL)} = \varphi(k, \delta, 0) < 1.$$

Hence, it holds that  $\varphi(k, \delta, p) \leq \varphi(k, \delta, 0) < 1$ . We now focus on  $\|\tilde{T}_1\|_\infty$  and  $\|\tilde{T}_2\|_\infty$ . Notice that  $\|\tilde{T}_1\|_\infty = \|\tilde{T}_2\|_\infty$  and

$$\begin{aligned} \|\tilde{T}_1\|_\infty &= \left| \frac{(k+p)e^{-kL} + (k-p)e^{kL}}{(k+p)e^{k(L+2\delta)} + (k-p)e^{-k(L+2\delta)}} \right| \\ &= \left| \frac{k \cosh(kL) - p \sinh(kL)}{k \cosh(k(L+2\delta)) + p \sinh(k(L+2\delta))} \right| < 1. \end{aligned}$$

262 In order to get a bound independently of  $k$ , we observe that  $\lim_{k \rightarrow \infty} \varphi(k, \delta, p) = \lim_{k \rightarrow \infty} \|\tilde{T}_1\|_\infty =$   
 263  $0$  if  $\delta > 0$ . Therefore defining  $\bar{\rho}(\delta) := \max_k \max\{\varphi(k, \delta, p), \|\tilde{T}_1(k, \delta, p)\|_\infty\}$ , we see that  
 264  $\|T_{2D}^O\|_\infty = \max\{\varphi, \|\tilde{T}_1\|, \|\tilde{T}_2\|\} < \bar{\rho}(\delta) < 1$ , for every  $k, \delta, p > 0$ .

265 Figure 5 (right) shows the behavior of the infinity norm and of the spectral radius of  $T_{2D}^O$   
 266 for a given value of  $p$ .

267 For the case without overlap, we need a further argument because for  $\delta = 0$  both  $\rho(T_{2D}^O)$   
 268 and  $\|T_{2D}^O\|_\infty$  are less than one for any finite frequency  $k$ , but tend to one as  $k \rightarrow \infty$ . One  
 269 can therefore construct a situation where the method would not be scalable as follows: sup-  
 270 pose we have  $N$  subdomains, and on the  $j$ -th subdomain we choose for the initial guess  $e_j^0$   
 271 the  $j$ -th frequency  $e_j^0 = \hat{e}_j^0 \sin(j \frac{\pi}{L} y)$ . Then the convergence of the method is determined by  
 272 the frequency which maximizes  $\rho(T_{2D}^O(k))$ . When the number of subdomains  $N$  becomes  
 273 large, this maximum is attained for the largest frequency  $k_N = N \frac{\pi}{L_y}$  since  $\rho(T_{2D}^O(k)) \rightarrow 1$  as  
 274  $k \rightarrow \infty$ . Thus, every time we add a subdomain to the chain with a new initial condition on  
 275 the interface  $N + 1$  according to our rule, the convergence rate of the method deteriorates  
 276 from  $\rho(T_{2D}^O(N \frac{\pi}{L}))$  to  $\rho(T_{2D}^O((N+1) \frac{\pi}{L}))$  and the scalability property is lost. Theorem 4 gives  
 277 however a sufficient condition such that the OSM is weakly scalable also without overlap,  
 278 and to see this we introduce the vector  $\mathbf{e}^n$  with  $e_k^n = \|\mathbf{r}^n(k)\|_\infty$  where  $\mathbf{r}^n(k)$ , defined in (21),  
 279 contains the Robin traces at the interfaces of the  $k$ -th Fourier mode.

280 **Theorem 4** *Given a tolerance  $\text{To1}$ , and supposing there exists a  $\tilde{k}$  that does not depend on*  
 281  *$N$  such that  $e_k^0 < \text{To1}$  for every  $k > \tilde{k}$ , then the OSM without overlap,  $\delta = 0$ , and  $p > 0$  is*  
 282 *weakly scalable.*

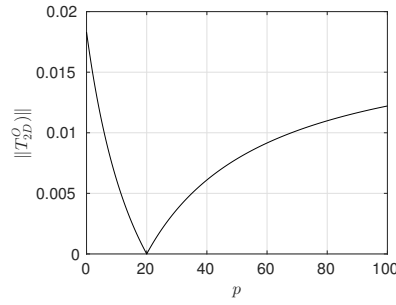
283 *Proof* Suppose that the initial guess satisfies  $\|\mathbf{e}^0\|_\infty > \text{To1}$ , since otherwise there is nothing  
 284 to prove. Then, due to the hypothesis, we have that  $\max_{\frac{\pi}{L} \leq k \leq \tilde{k}} e_k^0 > \text{To1}$ . We now show that  
 285 the method contracts with a  $\rho$  independent of the number of subdomains up to the tolerance  
 286  $\text{To1}$ , and therefore we have scalability. Indeed, for every  $k$  such that  $\frac{\pi}{L} \leq k \leq \tilde{k}$

$$e_k^n = \|\mathbf{r}^n(k)\|_\infty \leq \|T_{2D}^O(k)\|_\infty \|\mathbf{r}^{n-1}(k)\|_\infty \leq \|T_{2D}^O(\tilde{k})\|_\infty \|\mathbf{r}^{n-1}(k)\|_\infty = \|T_{2D}^O(\tilde{k})\|_\infty e_k^{n-1},$$

287 where  $\|T_{2D}^O(\tilde{k})\|_\infty = \max_{\frac{\pi}{L} \leq k \leq \tilde{k}} \|T_{2D}^O(k)\|_\infty < 1$  because  $\|T_{2D}^O(k)\|_\infty$  is strictly less than 1 for  
 288 every finite  $k$ . Now for  $k > \tilde{k}$ ,

$$e_k^n = \|\mathbf{r}^n(k)\|_\infty \leq \|T_{2D}^O(k)\|_\infty \|\mathbf{r}^{n-1}(k)\|_\infty \leq \|\mathbf{r}^{n-1}(k)\|_\infty = e_k^{n-1},$$

289 since  $\|T_{2D}^O(k)\|_\infty \leq 1$ . Therefore we observe that the method does not increase the error for  
 290 the frequencies  $k > \tilde{k}$  while it contracts for the other frequencies with a contraction factor  
 291 of at least  $\bar{\rho} = \|T_{2D}^O(\tilde{k})\|_\infty < 1$ . Hence, as long as  $\|\mathbf{e}^n\|_\infty > \text{To1}$ , we have  $\|\mathbf{e}^n\|_\infty \leq \bar{\rho}^n \|\mathbf{e}^0\|_\infty$   
 292 with  $\bar{\rho}$  independent of  $N$ .



**Fig. 6** Infinity norm of the iteration matrix  $T_{2D}^O$  as a function of  $p$  for  $L = 1, \widehat{L} = 1, \delta = 0.1, k = 20, N = 50$ .

293 Note that the technical assumption in Theorem 4 on the frequency content of the initial  
 294 error is not restrictive, since in a numerical implementation we have a maximum frequency  
 295  $k_{\max}$  which can be represented by the grid. Choosing  $\bar{k} = k_{\max}$ , the hypothesis of Theorem 4  
 296 is verified.

297 Note also that without overlap,  $\delta = 0$ , we have that  $\|T_{2D}^O\|_{\infty} = 1$  for  $p = 0$  or  $p \rightarrow \infty$ .  
 298 Therefore we can not conclude that the method is scalable in these two cases. For  $p = 0$ , the  
 299 OSM exchanges only partial derivatives information on the interface. For  $p \rightarrow \infty$ , we obtain  
 300 the classical Schwarz algorithm and it is well known [14] that without overlap ( $\delta = 0$ ), the  
 301 method does not converge.

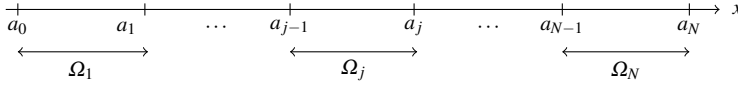
302 We finally show the behavior of  $p \mapsto \|T_{2D}^O(k, \delta, p)\|_{\infty}$  for a fixed pair  $(\delta, k)$  in Figure 6.  
 303 According to the proof of Theorem 3, the minimum of the function  $p \mapsto \varphi(k, \delta, p)$  is located  
 304 at  $p = k$ . Even though it is a minimum for  $\varphi(k, \delta, p)$  and not necessarily for  $\|T_{2D}^O(k, \delta, p)\|_{\infty}$   
 305 or  $\rho(T_{2D}^O)$ , we might deduce from Figure 6 that in order to eliminate the  $k$ -th frequency, a  
 306 good choice would be to set  $p := k$  in the OSM. For the Laplace equation, it has been shown  
 307 for two subdomains that setting  $p := k$  leads to a vanishing convergence factor  $\rho(k)$  for the  
 308 frequency  $k$ . In the case of many subdomains, a similar result has not been proved yet, but  
 309 Figure 6 indicates that it might hold as well.

## 310 5 Dirichlet-Neumann method

311 In this section, we study a parallel Dirichlet-Neumann method (PDNM) which, to the best  
 312 of our knowledge, has not been studied in the literature for a chain of  $N$  fixed-sized subdo-  
 313 mains. A discussion of this method for two subdomains is given in [2], see also [38] and [13,  
 314 page 717]. We now show that as for the Schwarz methods, the PDNM in 1D is not scalable,  
 315 while in 2D it is.

### 316 5.1 Dirichlet-Neumann method in 1D

317 Let us consider a set of domains  $\Omega_j = (a_{j-1}, a_j)$ , where  $a_j = jL$ . The subdomains have  
 318 length  $L$  and do not overlap. Such a non-overlapping decomposition of  $\Omega$  is shown in Figure  
 319 7, and corresponds to Figure 1 with  $\delta = 0$  and  $\bar{\Omega} = \cup_{j=1}^N \Omega_j$ . The error equations for PDNM



**Fig. 7** One-dimensional chain of  $N$  non-overlapping fixed-sized subdomains.

are given by

$$\begin{aligned} \partial_{xx}e_j^n &= 0 \text{ in } (a_{j-1}, a_j), \\ e_j^n(a_j) &= (1 - \theta)e_j^{n-1}(a_j) + \theta e_{j+1}^{n-1}(a_j), \\ \partial_x e_j^n(a_{j-1}) &= (1 - \lambda)\partial_x e_j^{n-1}(a_{j-1}) + \mu \partial_x e_{j-1}^{n-1}(a_{j-1}), \end{aligned} \quad (33)$$

for  $j = 2, \dots, N-1$ , and

$$\begin{aligned} \partial_{xx}e_1^n &= 0 \text{ in } (a_1, a_1), \\ e_1^n(a_0) &= 0, \\ e_1^n(a_1) &= (1 - \theta)e_1^{n-1}(a_1) + \theta e_2^{n-1}(a_1), \end{aligned} \quad (34)$$

and

$$\begin{aligned} \partial_{xx}e_N^n &= 0 \text{ in } (a_{N-1}, a_N), \\ \partial_x e_N^n(a_{N-1}) &= (1 - \mu)\partial_x e_N^{n-1}(a_{N-1}) + \mu \partial_x e_{N-1}^{n-1}(a_{N-1}), \\ e_N^n(a_N) &= 0. \end{aligned} \quad (35)$$

In (33)-(34),  $\theta$  and  $\mu$  are relaxation parameters in  $(0, 1)$ . Now, we define

$$\mathcal{D}_j^n := e_j^n(a_j), \quad \mathcal{N}_j^n := \partial_x e_j^n(a_{j-1}),$$

and by a direct calculation we find that the solution to (33) is given by

$$e_j^n(x) = \mathcal{N}_j^n(x - a_j) + \mathcal{D}_j^n,$$

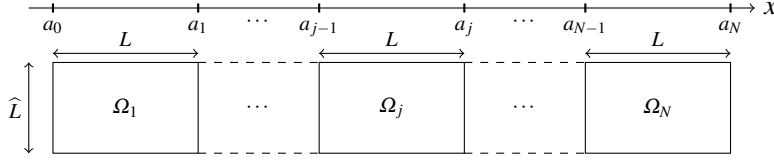
for  $j = 2, \dots, N-1$ , and

$$e_1^n(x) = \frac{\mathcal{D}_1^n}{L}(x - a_0), \quad e_N^n(x) = \mathcal{N}_N^n(x - a_N).$$

Introducing these expressions into the transmission conditions in (33), we get

$$\begin{aligned} \begin{bmatrix} \mathbf{0} \\ \mathcal{D}_1^n \end{bmatrix} &= \widehat{T}_1 \begin{bmatrix} \mathcal{N}_1^{n-1} \\ \mathcal{D}_1^{n-1} \end{bmatrix} + T_2 \begin{bmatrix} \mathcal{N}_2^{n-1} \\ \mathcal{D}_2^{n-1} \end{bmatrix}, \\ \begin{bmatrix} \mathcal{N}_2^n \\ \mathcal{D}_2^n \end{bmatrix} &= \widetilde{T}_0 \begin{bmatrix} \mathbf{0} \\ \mathcal{D}_1^{n-1} \end{bmatrix} + T_1 \begin{bmatrix} \mathcal{N}_2^{n-1} \\ \mathcal{D}_2^{n-1} \end{bmatrix} + T_2 \begin{bmatrix} \mathcal{N}_3^{n-1} \\ \mathcal{D}_3^{n-1} \end{bmatrix}, \\ \begin{bmatrix} \mathcal{N}_j^n \\ \mathcal{D}_j^n \end{bmatrix} &= T_0 \begin{bmatrix} \mathcal{N}_{j-1}^{n-1} \\ \mathcal{D}_{j-1}^{n-1} \end{bmatrix} + T_1 \begin{bmatrix} \mathcal{N}_j^{n-1} \\ \mathcal{D}_j^{n-1} \end{bmatrix} + T_2 \begin{bmatrix} \mathcal{N}_{j+1}^{n-1} \\ \mathcal{D}_{j+1}^{n-1} \end{bmatrix}, \text{ for } j = 3, \dots, N-2, \\ \begin{bmatrix} \mathcal{N}_{N-1}^n \\ \mathcal{D}_{N-1}^n \end{bmatrix} &= T_0 \begin{bmatrix} \mathcal{N}_{N-2}^{n-1} \\ \mathcal{D}_{N-2}^{n-1} \end{bmatrix} + T_1 \begin{bmatrix} \mathcal{N}_{N-1}^{n-1} \\ \mathcal{D}_{N-1}^{n-1} \end{bmatrix} + \widetilde{T}_2 \begin{bmatrix} \mathcal{N}_N^{n-1} \\ \mathbf{0} \end{bmatrix}, \\ \begin{bmatrix} \mathcal{N}_N^n \\ \mathbf{0} \end{bmatrix} &= \widetilde{T}_1 \begin{bmatrix} \mathcal{N}_N^{n-1} \\ \mathcal{D}_N^{n-1} \end{bmatrix} + \widetilde{T}_2 \begin{bmatrix} \mathcal{N}_{N-1}^{n-1} \\ \mathcal{D}_{N-1}^{n-1} \end{bmatrix}, \end{aligned} \quad (36)$$





**Fig. 9** Non overlapping domain decomposition in two dimensions. Notice that  $a_j = jL$ .

### 330 5.2 Dirichlet-Neumann method in 2D

We consider now the two dimensional problem whose non-overlapping domain decomposition is shown in Figure 9, which corresponds to Figure 2 with  $\delta = 0$ . The PDNM is given by

$$\begin{aligned} -\Delta e_j^n &= 0 \quad \text{in } \Omega_j, \\ e_j^n(\cdot, 0) &= 0, \quad e_j^n(\cdot, \widehat{L}) = 0, \\ e_j^n(a_j, \cdot) &= (1 - \theta)e_j^{n-1}(a_j, \cdot) + \theta e_{j+1}^{n-1}(a_j, \cdot), \\ \partial_x e_j^n(a_{j-1}, \cdot) &= (1 - \mu)\partial_x e_j^{n-1}(a_{j-1}, \cdot) + \mu \partial_x e_{j-1}^{n-1}(a_{j-1}, \cdot), \end{aligned}$$

for  $j = 2, \dots, N-1$ , and

$$\begin{aligned} -\Delta e_1^n &= 0 \quad \text{in } \Omega_1, \\ e_1^n(\cdot, 0) &= 0, \quad e_1^n(\cdot, \widehat{L}) = 0, \\ e_1^n(a_0, \cdot) &= 0, \\ e_1^n(a_1, \cdot) &= (1 - \theta)e_1^{n-1}(a_1, \cdot) + \theta e_2^{n-1}(a_1, \cdot), \end{aligned}$$

and

$$\begin{aligned} -\Delta e_N^n &= 0 \quad \text{in } \Omega_N, \\ e_N^n(\cdot, 0) &= 0, \quad e_N^n(\cdot, \widehat{L}) = 0, \\ \partial_x e_N^n(a_{N-1}, \cdot) &= (1 - \mu)\partial_x e_N^{n-1}(a_{N-1}, \cdot) + \mu \partial_x e_{N-1}^{n-1}(a_{N-1}, \cdot), \\ e_N^n(a_N, \cdot) &= 0, \end{aligned}$$

where  $\theta, \mu \in (0, 1)$ . Now, we consider the Fourier expansion of  $e_j^n$  as in the previous sections. Since the Fourier coefficients  $v_j^n(x, k)$  solve

$$\begin{aligned} \partial_{xx} v_j^n &= k^2 v_j^n \quad \text{in } (a_j, b_j), \\ v_j^n(a_j) &= (1 - \theta)v_j^{n-1}(a_j) + \theta v_{j+1}^{n-1}(a_j), \\ \partial_x v_j^n(a_{j-1}) &= (1 - \mu)\partial_x v_j^{n-1}(a_{j-1}) + \mu \partial_x v_{j-1}^{n-1}(a_{j-1}), \end{aligned}$$

defining

$$\begin{aligned} \mathcal{D}_j^n &:= (1 - \theta)v_j^{n-1}(a_j) + \theta v_{j+1}^{n-1}(a_j), \\ \mathcal{N}_j^n &:= (1 - \mu)\partial_x v_j^{n-1}(a_{j-1}) + \mu \partial_x v_{j-1}^{n-1}(a_{j-1}), \end{aligned}$$

we get

$$v_j^n(x, k) = \frac{1}{k\gamma_2} \left[ ke^{-k[(j-1)L-x]} \mathcal{D}_j^n + e^{-k(jL-x)} \mathcal{N}_j^n + ke^{k[(j-1)L-x]} \mathcal{D}_j^n - e^{k(jL-x)} \mathcal{N}_j^n \right],$$

for  $j = 2, \dots, N-1$ , and

$$v_1^n(x, k) = \frac{D_1^n}{\gamma_1} [e^{kx} - e^{-kx}], \quad v_N^n(x, k) = \frac{1}{k\gamma_2} \left[ e^{-k(NL-x)} N_N^n - e^{k(NL-x)} N_N^n \right],$$

331 where  $\gamma_1 := e^{-kL} - e^{kL}$  and  $\gamma_2 := e^{kL} + e^{-kL}$ . Exploiting the definition of  $\mathcal{N}_j^n$  and  $\mathcal{D}_j^n$ , we  
332 get

$$\begin{aligned} \begin{bmatrix} \mathbf{0} \\ \mathcal{D}_1^n \end{bmatrix} &= \widehat{T}_1 \begin{bmatrix} \mathcal{N}_1^{n-1} \\ \mathcal{D}_1^{n-1} \end{bmatrix} + T_2 \begin{bmatrix} \mathcal{N}_2^{n-1} \\ \mathcal{D}_2^{n-1} \end{bmatrix}, \\ \begin{bmatrix} \mathcal{N}_2^n \\ \mathcal{D}_2^n \end{bmatrix} &= \widetilde{T}_0 \begin{bmatrix} \mathbf{0} \\ \mathcal{D}_1^{n-1} \end{bmatrix} + T_1 \begin{bmatrix} \mathcal{N}_2^{n-1} \\ \mathcal{D}_2^{n-1} \end{bmatrix} + T_2 \begin{bmatrix} \mathcal{N}_3^{n-1} \\ \mathcal{D}_3^{n-1} \end{bmatrix}, \\ \begin{bmatrix} \mathcal{N}_j^n \\ \mathcal{D}_j^n \end{bmatrix} &= T_0 \begin{bmatrix} \mathcal{N}_{j-1}^{n-1} \\ \mathcal{D}_{j-1}^{n-1} \end{bmatrix} + T_1 \begin{bmatrix} \mathcal{N}_j^{n-1} \\ \mathcal{D}_j^{n-1} \end{bmatrix} + T_2 \begin{bmatrix} \mathcal{N}_{j+1}^{n-1} \\ \mathcal{D}_{j+1}^{n-1} \end{bmatrix}, \quad \text{for } j = 3, \dots, N-2, \quad (38) \\ \begin{bmatrix} \mathcal{N}_{N-1}^n \\ \mathcal{D}_{N-1}^n \end{bmatrix} &= T_0 \begin{bmatrix} \mathcal{N}_{N-2}^{n-1} \\ \mathcal{D}_{N-2}^{n-1} \end{bmatrix} + T_1 \begin{bmatrix} \mathcal{N}_{N-1}^{n-1} \\ \mathcal{D}_{N-1}^{n-1} \end{bmatrix} + \widetilde{T}_2 \begin{bmatrix} \mathcal{N}_N^{n-1} \\ \mathbf{0} \end{bmatrix}, \\ \begin{bmatrix} \mathcal{N}_N^n \\ \mathbf{0} \end{bmatrix} &= \widetilde{T}_1 \begin{bmatrix} \mathcal{N}_N^{n-1} \\ \mathcal{D}_N^{n-1} \end{bmatrix} + \widetilde{T}_2 \begin{bmatrix} \mathcal{N}_{N-1}^{n-1} \\ \mathcal{D}_{N-1}^{n-1} \end{bmatrix}, \end{aligned}$$

where

$$\begin{aligned} T_0 &:= \begin{bmatrix} \frac{2}{\gamma_2} & \frac{k\gamma_1}{\gamma_2} \\ 0 & 0 \end{bmatrix}, \quad T_1 := \begin{bmatrix} 1-\mu & 0 \\ 0 & 1-\theta \end{bmatrix}, \quad T_2 := \begin{bmatrix} 0 & 0 \\ -\frac{\theta\gamma_1}{k\gamma_2} & \frac{2\theta}{\gamma_2} \end{bmatrix}, \\ \widetilde{T}_0 &:= \begin{bmatrix} 0 & \frac{\mu k\gamma_2}{\gamma_1} \\ 0 & 0 \end{bmatrix}, \quad \widehat{T}_1 := \begin{bmatrix} 0 & 0 \\ 0 & 1-\theta \end{bmatrix}, \quad \widetilde{T}_1 := \begin{bmatrix} 1-\mu & 0 \\ 0 & 0 \end{bmatrix}, \quad \widetilde{T}_2 := \begin{bmatrix} 0 & 0 \\ -\frac{\theta\gamma_1}{k\gamma_2} & 0 \end{bmatrix}. \end{aligned}$$

Defining  $\mathbf{e}^n := [0, \mathcal{D}_1^n, \mathcal{N}_2^n, \mathcal{D}_2^n, \dots, \mathcal{N}_j^n, \mathcal{D}_j^n, \dots, \mathcal{N}_{N-1}^n, \mathcal{D}_{N-1}^n, \mathcal{N}_N^n, 0]^\top$ , the iteration relations (38) may be rewritten as

$$\mathbf{e}^n = T_{2D}^{DN} \mathbf{e}^{n-1},$$

333 where  $T_{2D}^{DN}$  has the same structure as  $T_{1D}^{DN}$  given in (37).

334 Even though we observe numerically that  $\rho(T_{2D}^{DN}) < 1$ , one can also verify that in general  
335  $\|T_{2D}^{DN}\|_\infty > 1$ . Hence, in contrast to the other methods discussed in this paper, the infinity-  
336 norm is not suitable to bound the spectral radius and conclude convergence and scalability.  
337 Nevertheless in Theorem 5, under certain assumptions and using similarity arguments as in  
338 [6], we prove scalability of the PDNM.

**Theorem 5** Denote by  $k_{\min}$  the minimum frequency and define  $\alpha(x) := 1/\cosh(x)$ . If  $\theta = \mu$ , then

$$\rho(T_{2D}^{DN}) \leq \bar{\rho}(\mu) := \sqrt{1 - \mu + \mu^2} + \mu\alpha(k_{\min}L),$$

339 where  $\bar{\rho}(\mu)$  is independent of  $N$ . Furthermore, if  $\cosh(k_{\min}L) > 2$ , then  $\bar{\rho}(\mu) < 1$  for any  
340 positive  $\mu$  such that  $\mu < \frac{1-2\alpha(k_{\min}L)}{1-\alpha(k_{\min}L)^2}$ , which implies that the PDNM is convergent and scal-  
341 able.







356 and hence  $\sqrt{\rho(T_{\text{off}}^\top T_{\text{off}})} = \frac{2\mu}{\gamma_2}$ . Now, we focus on the term  $\rho(T_{\text{diag}}^\top T_{\text{diag}})$ . The block diagonal  
 357 structure of  $T_{\text{diag}}^\top T_{\text{diag}}$  allows us to write

$$\rho(T_{\text{diag}}^\top T_{\text{diag}}) = \sqrt{\max\{\rho(\tilde{C}^\top \tilde{C}), \rho(\hat{C}^\top \hat{C}), \rho(\bar{C}^\top \bar{C})\}}. \quad (40)$$

The evaluation of the spectral radii  $\rho(\tilde{C}^\top \tilde{C})$ ,  $\rho(\hat{C}^\top \hat{C})$ , and  $\rho(\bar{C}^\top \bar{C})$  leads to the analysis of cumbersome formulas, and we thus bound instead the spectral radii by the corresponding infinity-norms. To do so, setting  $\tilde{d}_1 := \gamma_1$  and  $\tilde{d}_2 := k\gamma_2$ , we obtain

$$\rho(\tilde{C}^\top \tilde{C}) = \rho(\tilde{G}\tilde{B}^\top \tilde{G}^{-1} \tilde{G}^{-1} \tilde{B}\tilde{G}) \leq \|\tilde{G}\tilde{B}^\top \tilde{G}^{-1} \tilde{G}^{-1} \tilde{B}\tilde{G}\|_\infty = 2\mu^2 - 2\mu + 1.$$

Next, we set  $\hat{d}_1 := \gamma_2$  and  $\hat{d}_2 := k\gamma_1$  and get

$$\begin{aligned} \rho(\hat{C}^\top \hat{C}) &= \rho(\hat{G}\hat{B}^\top \hat{G}^{-1} \hat{G}^{-1} \hat{B}\hat{G}) \leq \|\hat{G}\hat{B}^\top \hat{G}^{-1} \hat{G}^{-1} \hat{B}\hat{G}\|_\infty \\ &= 2\mu^2 - 2\mu + 1 + \frac{4\mu(1-\mu)}{\gamma_2^2} \leq 2\mu^2 - 2\mu + 1 + \frac{4\mu(1-\mu)}{(e^{k_{\min}L} + e^{-k_{\min}L})^2}, \end{aligned}$$

where we used that  $\gamma_2 = e^{kL} + e^{-kL} \geq e^{k_{\min}L} + e^{-k_{\min}L}$  for any  $k \geq k_{\min}$ , and

$$\begin{aligned} \rho(\bar{C}^\top \bar{C}) &= \rho(\bar{G}\bar{B}^\top \bar{G}^{-1} \bar{G}^{-1} \bar{B}\bar{G}) \leq \|\bar{G}\bar{B}^\top \bar{G}^{-1} \bar{G}^{-1} \bar{B}\bar{G}\|_\infty \\ &= \max \left\{ 1 - \mu, 1 - \mu + \frac{\mu^2(e^{-kL} - e^{kL})^4}{(e^{-kL} + e^{kL})^4} \right\} \leq 1 - \mu + \mu^2, \end{aligned}$$

where the fact that  $\frac{(e^{-kL} - e^{kL})^4}{(e^{-kL} + e^{kL})^4} \leq 1$  for any  $k$  is used. Now, a direct calculation shows that

$$2\mu^2 - 2\mu + 1 \leq 2\mu^2 - 2\mu + 1 + \frac{4\mu(1-\mu)}{(e^{k_{\min}L} + e^{-k_{\min}L})^2} \leq 1 - \mu + \mu^2,$$

for any  $\mu \in (0, 1)$ . Therefore, we obtain

$$\|T_{\text{diag}}\|_2 = \rho(T_{\text{diag}}^\top T_{\text{diag}}) \leq \sqrt{1 - \mu + \mu^2}.$$

Recalling (39) and (40), we conclude that

$$\begin{aligned} \rho(T_{2D}^{DN}) &\leq \|T_{\text{diag}}\|_2 + \|T_{\text{off}}\|_2 \leq \sqrt{1 - \mu + \mu^2} + \frac{2\mu}{\gamma_2} \\ &\leq \sqrt{1 - \mu + \mu^2} + \frac{2\mu}{(e^{k_{\min}L} + e^{-k_{\min}L})} =: \bar{\rho}(\mu), \end{aligned}$$

358 which is first statement of the theorem. The second part follows now from Lemma 3 by  
 359 observing that if  $\bar{\rho}(\mu) < 1$ , then  $\rho(T_{2D}^{DN}) \leq \bar{\rho}(\mu) < 1$  where  $\bar{\rho}(\mu)$  is independent of  $N$ .

360 **6 Neumann-Neumann method**

In this section, we study the convergence of the Neumann-Neumann method (NNM) as described in [40] for the solution of the two-dimensional problem (4)-(5)<sup>1</sup>. The error equations for NNM are given by the following: first solve

$$\begin{aligned} -\Delta e_j^n &= 0 \text{ in } \Omega_j, \\ e_j^n(\cdot, 0) &= 0, \quad e_j^n(\cdot, L) = 0, \\ e_j^n(a_{j-1}, \cdot) &= \mathcal{D}_{j-1}^n, \quad e_j^n(a_j, \cdot) = \mathcal{D}_j^n, \end{aligned}$$

for  $j = 2, \dots, N-1$  and

$$\begin{aligned} -\Delta e_1^n &= 0 \text{ in } \Omega_1, & -\Delta e_N^n &= 0 \text{ in } \Omega_N, \\ e_1^n(\cdot, 0) &= 0, \quad e_1^n(\cdot, L) = 0, & e_N^n(\cdot, 0) &= 0, \quad e_N^n(\cdot, L) = 0, \\ e_1^n(a_0, \cdot) &= 0, \quad e_1^n(a_1, \cdot) = \mathcal{D}_1^n, & e_N^n(a_{N-1}, \cdot) &= \mathcal{D}_{N-1}^n, \quad e_N^n(a_N, \cdot) = 0, \end{aligned}$$

then solve

$$\begin{aligned} -\Delta \psi_j^n &= 0 \text{ in } \Omega_j, \\ \partial_x \psi_j^n(\cdot, 0) &= 0, \quad \psi_j^n(\cdot, L) = 0, \\ \partial_x \psi_j^n(a_{j-1}, \cdot) &= \partial_x e_j^n(a_{j-1}, \cdot) - \partial_x e_{j-1}^n(a_{j-1}, \cdot), \\ \partial_x \psi_j^n(a_j, \cdot) &= \partial_x e_j^n(a_j, \cdot) - \partial_x e_{j+1}^n(a_j, \cdot), \end{aligned}$$

for  $j = 2, \dots, N-1$  and

$$\begin{aligned} -\Delta \psi_1^n &= 0 \text{ in } \Omega_1, \\ \psi_1^n(\cdot, 0) &= 0, \quad \psi_1^n(\cdot, L) = 0, \quad \psi_1^n(a_0, \cdot) = 0, \\ \partial_x \psi_1^n(a_1, \cdot) &= \partial_x e_1^n(a_1, \cdot) - \partial_x e_2^n(a_1, \cdot), \end{aligned}$$

and

$$\begin{aligned} -\Delta \psi_N^n &= 0 \text{ in } \Omega_N, \\ \psi_N^n(\cdot, 0) &= 0, \quad \psi_N^n(\cdot, L) = 0, \quad \psi_N^n(a_N, \cdot) = 0, \\ \partial_x \psi_N^n(a_{N-1}, \cdot) &= \partial_x e_N^n(a_{N-1}, \cdot) - \partial_x e_{N-1}^n(a_{N-1}, \cdot), \end{aligned}$$

361 and finally set

$$\mathcal{D}_j^{n+1} := \mathcal{D}_j^n - \vartheta(\psi_{j+1}^n(a_j, \cdot) + \psi_j^n(a_j, \cdot)), \quad (41)$$

for  $j = 1, \dots, N-1$ , where  $\vartheta > 0$ . As in the last sections, we use the Fourier expansion

$$e_j^n(x, y) = \sum_{m=1}^{\infty} v_j^n(x, k) \sin(ky), \quad \psi_j^n(x, y) = \sum_{m=1}^{\infty} w_j^n(x, k) \sin(ky),$$

where  $k = \frac{m\pi}{L}$ . The Fourier coefficients  $v_j^n(x, k)$  and  $w_j^n(x, k)$  solve the problems

$$\begin{aligned} k^2 v_j^n - \partial_{xx} v_j^n &= 0 \text{ in } (a_{j-1}, a_j), & k^2 w_j^n - \partial_{xx} w_j^n &= 0 \text{ in } (a_{j-1}, a_j), \\ v_j^n(a_{j-1}, k) &= \mathcal{D}_{j-1}^n, & \partial_x w_j^n(a_{j-1}, k) &= \partial_x v_j^n(a_{j-1}, k) - \partial_x v_{j-1}^n(a_{j-1}, k), \\ v_j^n(a_j, k) &= \mathcal{D}_j^n, & \partial_x w_j^n(a_j, k) &= \partial_x v_j^n(a_j, k) - \partial_x v_{j+1}^n(a_j, k), \end{aligned}$$

<sup>1</sup> Notice that in 1D the NNM is not well defined because the solution of pure Neumann problems with a non-zero kernel are necessary for the interior subdomains.

for  $j = 2, \dots, N-1$ , and

$$\begin{aligned} k^2 v_1^n - \partial_{xx} v_1^n &= 0 \quad \text{in } (a_0, a_1), & k^2 w_1^n - \partial_{xx} w_1^n &= 0 \quad \text{in } (a_0, a_1), \\ v_1^n(a_0, k) &= 0, & \tilde{w}_1^n(a_0, k) &= 0, \\ v_1^n(a_1, k) &= \mathcal{D}_1^n, & \partial_x w_1^n(a_1, k) &= \partial_x v_1^n(a_1, k) - \partial_x v_2^n(a_1, k), \end{aligned}$$

and

$$\begin{aligned} k^2 v_N^n - \partial_{xx} v_N^n &= 0 \quad \text{in } (a_{N-1}, a_N), & k^2 w_N^n - \partial_{xx} w_N^n &= 0 \quad \text{in } (a_{N-1}, a_N), \\ v_N^n(a_{N-1}, k) &= \mathcal{D}_{N-1}^n, & \partial_x w_N^n(a_{N-1}, k) &= \partial_x v_N^n(a_{N-1}, k) - \partial_x v_{N-1}^n(a_{N-1}, k), \\ v_N^n(a_N, k) &= 0, & w_N^n(a_N, k) &= 0, \end{aligned}$$

for the first and last subdomains. Setting for simplicity of notation  $\mathcal{D}_0^n = \mathcal{D}_N^n = 0$  and defining  $\gamma_1 := e^{kL} - e^{-kL}$ , the solution  $v_j^n$  can be written as

$$v_j^n(x, k) = \frac{1}{\gamma_1} \left[ \mathcal{D}_j^n \left( e^{k(x-(j-1)L)} - e^{k((j-1)L-x)} \right) + \mathcal{D}_{j-1}^n \left( e^{k(jL-x)} - e^{k(x-jL)} \right) \right],$$

which is used to solve the problems in  $w_j^n$ , and we obtain

$$\begin{aligned} w_j^n(x, k) &= \frac{1}{\gamma_1^2} \left( 2\mathcal{D}_{j-1}^n (e^{kL} + e^{-kL}) - 2\mathcal{D}_j^n - 2\mathcal{D}_{j-2}^n \right) \left( e^{k(x-jL)} + e^{k(jL-x)} \right) \\ &\quad + \frac{1}{\gamma_1^2} \left( 2\mathcal{D}_j^n (e^{kL} + e^{-kL}) - 2\mathcal{D}_{j-1}^n - 2\mathcal{D}_{j+1}^n \right) \left( e^{k(x-(j-1)L)} + e^{k((j-1)L-x)} \right), \end{aligned}$$

for  $j = 2, \dots, N-1$ , and

$$\begin{aligned} w_1^n(x, k) &= \frac{1}{\gamma_1 \gamma_2} \left( 2\mathcal{D}_1^n (e^{kL} + e^{-kL}) - 2\mathcal{D}_2^n \right) \left( e^{kx} - e^{-kx} \right), \\ w_N^n(x, k) &= \frac{1}{\gamma_1 \gamma_2} \left( -2\mathcal{D}_{N-1}^n (e^{kL} + e^{-kL}) + 2\mathcal{D}_{N-2}^n \right) \left( e^{k(x-NL)} - e^{k(NL-x)} \right), \end{aligned}$$

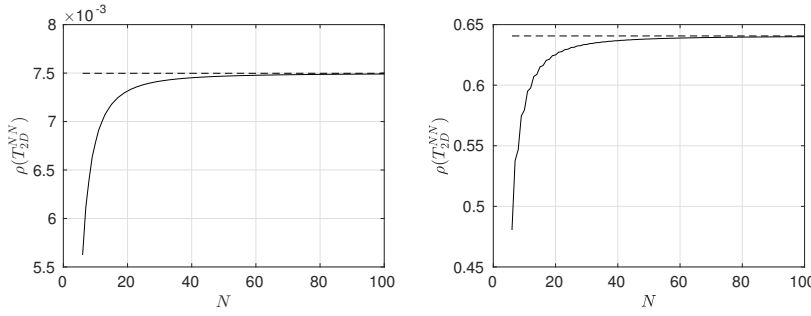
362 where  $\gamma_2 := e^{kL} + e^{-kL}$ . Using equation (41) we get

$$\mathcal{D}_j^{n+1} = \mathcal{D}_j^n - \frac{\vartheta}{\gamma_1^2} \left[ 4\mathcal{D}_j^n \left( (e^{kL} + e^{-kL})^2 - 2 \right) - 4\mathcal{D}_{j-2}^n - 4\mathcal{D}_{j+2}^n \right], \quad (42)$$

363 for  $j = 2, \dots, N-2$ , and

$$\begin{aligned} \mathcal{D}_1^{n+1} &= \mathcal{D}_1^n - \frac{\vartheta}{\gamma_2} \left( 2(e^{kL} + e^{-kL})\mathcal{D}_1^n - 2\mathcal{D}_2^n \right) \\ &\quad - \frac{\vartheta}{\gamma_1^2} \left( 2((e^{kL} + e^{-kL})^2 - 2)\mathcal{D}_1^n + 2(e^{kL} + e^{-kL})\mathcal{D}_2^n - 4\mathcal{D}_3^n \right), \\ \mathcal{D}_{N-1}^{n+1} &= \mathcal{D}_{N-1}^n - \frac{\vartheta}{\gamma_2} \left( 2(e^{kL} + e^{-kL})\mathcal{D}_{N-2}^n - 2\mathcal{D}_{N-2}^n \right) \\ &\quad - \frac{\vartheta}{\gamma_1^2} \left( 2((e^{kL} + e^{-kL})^2 - 2)\mathcal{D}_{N-1}^n + 2(e^{kL} + e^{-kL})\mathcal{D}_{N-2}^n - 4\mathcal{D}_{N-3}^n \right). \end{aligned} \quad (43)$$



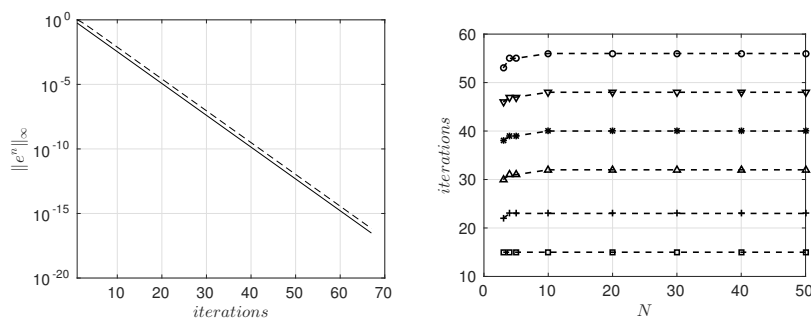


**Fig. 11** Spectral radius (solid line) and infinity-norm (dashed line) of  $T_{2D}^{NN}$  for  $L = 1$ ,  $\vartheta = \frac{1}{4}$ , and  $k = \pi$ . Left:  $\widehat{L} = 1$ . Right:  $\widehat{L} = 3$ . We see that the subdomain height has a strong influence on the performance.

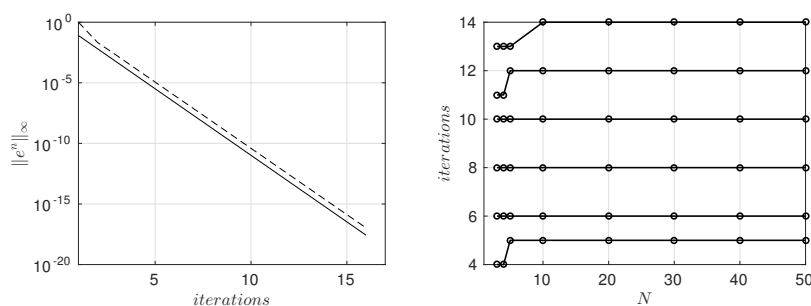
## 377 7 Numerical experiments

378 We solve numerically problem (4)-(5) with  $f_j = 0$  and  $g_j = 0$  by applying the domain-  
 379 decomposition methods studied in the previous sections. We choose subdomains having  
 380 height  $\widehat{L} = 1$  and length  $L = 1$  (without overlap), that is each subdomain without including  
 381 the overlap is a unit square. The Laplace operator defined on this square is discretized by  
 382 the classical 5-point finite-difference stencil defined on a uniform grid with  $J$  interior points  
 383 in both  $x$  and  $y$  directions, with  $J = 100$ . The mesh size is  $h = \frac{1}{J+1}$  and the overlap (for  
 384 PSM and OSM) is set to  $\delta = 10h$ . The number of (fixed-sized) subdomains is  $N = 100$ .  
 385 We generate the error sequence  $\{e_j^n\}_n$  by applying PSM, OSM, PDNM, and NNM starting  
 386 with an initial error  $e^0(x, y) = \sum_{m=1}^J \gamma_m \sin(m\pi y)$ , where the coefficients  $\gamma_m$  are randomly  
 387 chosen in the interval  $(-1, 1)$  in order to insert error components in all the frequencies. For  
 388 the OSM the optimized Robin parameter is  $p = 3.61$ , which has been found minimizing  
 389 the maximum with respect to  $k$  of the spectral radii of the matrices  $T_{2D}^O$ . The relaxation  
 390 parameters of the PDNM are  $\theta = \mu = \frac{1}{2}$ , while the relaxation parameter of the NNM is  
 391  $\theta = \frac{1}{4}$ . The iterative procedures are stopped when the error  $\|e^n\|_\infty := \max_j \max_{\Omega_j} |e_j|$   
 392 is smaller than the tolerance  $\tau_{\text{tol}} = 10^{-16}$ . In Figures 12-13-14-15 (left) we compare the decay  
 393 of the errors of the 4 methods studied in this paper with the theoretical convergence rate  
 394 obtained by a numerical estimate of the spectral radii of the transfer matrices  $T_{2D}$ ,  $T_{2D}^O$ ,  $T_{2D}^{DN}$ ,  
 395 and  $T_{2D}^{NN}$ .

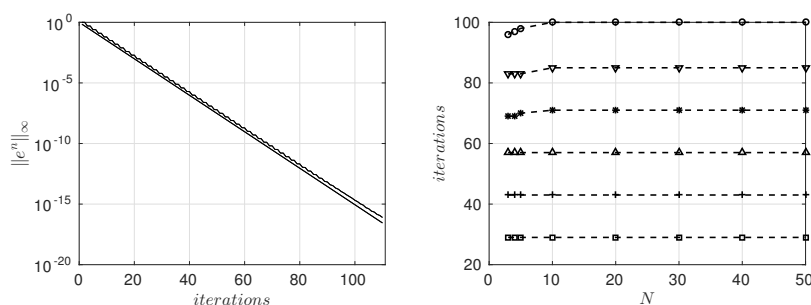
396 In particular, the spectral radii are computed using their maximizing frequencies, that  
 397 is  $k = k_{\min} = \pi$  for all the methods. In all cases we observe a very good agreement of the  
 398 numerical decay (dashed lines) with the theoretical estimate (solid lines). We see also that  
 399 the NNM requires less iterations (only 7) than all the others to reach the desired tolerance.  
 400 The OSM requires about 16 iterations to converge, but at each iteration only  $J$  subproblems  
 401 are solved, while the NNM requires the solution of  $2J$  subproblems, so their performance is  
 402 comparable, and in addition, one could use higher order optimized transmission conditions  
 403 for OSM, see [13], to lower the iteration count further. The PSM and the PDNM converge  
 404 more slowly, needing about 65 and 110 iterations. Finally, in order to study the scalability  
 405 of the 4 methods, we repeat the previous experiment with different numbers of fixed-sized  
 406 subdomains  $N$  and different values of  $\text{tol}$ . The results shown in Figures 12-13-14-15 (right)  
 407 show that the number of iterations (up to small changes for small values of  $N$ ) is constant  
 408 with respect to  $N$ . These numerical experiments are in agreement with the theoretical results  
 409 proved in this paper.



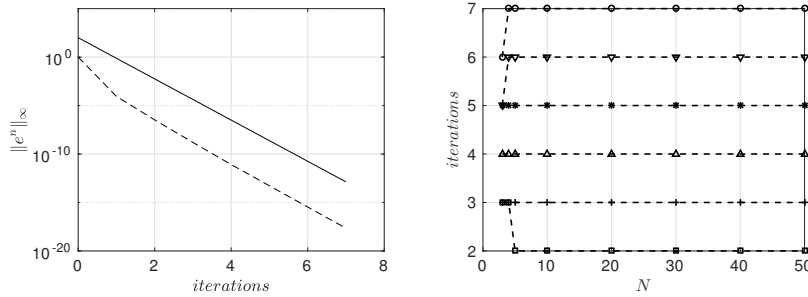
**Fig. 12** Left: numerical (dashed line) and theoretical (solid line) decay of the error of the PSM. Right: number of iterations performed as function of the number of subdomains  $N$ ; each curve corresponds to a different fixed tolerance. In particular, from the bottom to the top the curves correspond to tol equal to  $10^{-4}$ ,  $10^{-6}$ ,  $10^{-8}$ ,  $10^{-10}$ ,  $10^{-12}$ ,  $10^{-14}$ .



**Fig. 13** Left: numerical (dashed line) and theoretical (solid line) decay of the error of the OSM. Right: number of iterations performed as function of the number of subdomains  $N$ ; each curve corresponds to a different fixed tolerance. In particular, from the bottom to the top the curves corresponds to tol equal to  $10^{-4}$ ,  $10^{-6}$ ,  $10^{-8}$ ,  $10^{-10}$ ,  $10^{-12}$ ,  $10^{-14}$ .



**Fig. 14** Left: numerical (dashed line) and theoretical (solid line) decay of the error of the PDNM. Right: number of subdomains  $N$ ; each curve corresponds to a different fixed tolerance. In particular, from the bottom to the top the curves corresponds to tol equal to  $10^{-4}$ ,  $10^{-6}$ ,  $10^{-8}$ ,  $10^{-10}$ ,  $10^{-12}$ ,  $10^{-14}$ .



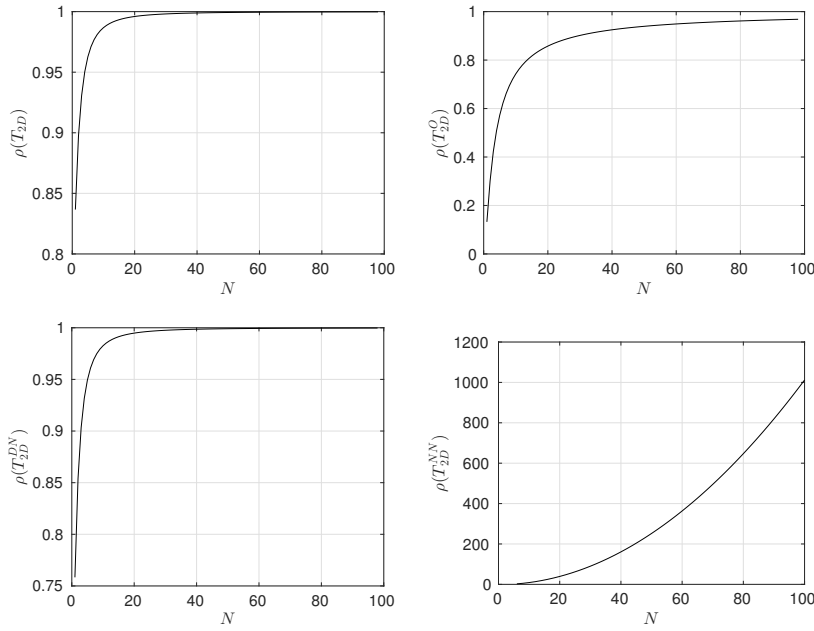
**Fig. 15** Left: numerical (dashed line) and theoretical (solid line) decay of the error of the NNM. Right: number of iterations performed as function of the number of subdomains  $N$ ; each curve corresponds to a different fixed tolerance. In particular, from the bottom to the top the curves corresponds to tol equal to  $10^{-4}$ ,  $10^{-6}$ ,  $10^{-8}$ ,  $10^{-10}$ ,  $10^{-12}$ ,  $10^{-14}$ .

## 410 8 Why the methods scale in 2D but not in 1D

411 We showed a very different convergence behavior for all one level domain-decomposition  
 412 methods for the solution of a chain of  $N$  fixed-sized subdomains when  $N$  increases: the  
 413 methods for the solution of a one-dimensional chain are not scalable, whereas they are scal-  
 414 able for the solution of a two-dimensional chain. At first glance, the two models seem to be  
 415 very similar, and we want to give now an intuitive explanation for this different behavior.  
 416 As we have already discussed in Section 3.1 for the PSM in the one-dimensional case, the  
 417 propagation of a reduction of the error starts from the first and last subdomains and moves  
 418 towards the subdomains being in the middle of the chain. Therefore, for some given initial  
 419 error  $e^0$ , one has to wait about  $N/2$  iterations before observing a contraction of the error in  
 420 the middle of the chain. This fact is due to the (only) two homogeneous Dirichlet boundary  
 421 conditions that are imposed at the extrema  $x = a_1$  and  $x = b_N$  of the domain  $\Omega$ , see (6)-(7).  
 422 Therefore, the “internal subdomains” do not directly benefit from the good effect of these  
 423 zero Dirichlet conditions. On the other hand, in the two-dimensional case, each subdomain  
 424 in the chain benefits from the zero Dirichlet conditions imposed at the top and at the bottom  
 425 of the rectangles  $\Omega_j$ , see (9)-(10). Therefore, a contraction of the error starts immediately in  
 426 each subdomain and one has not to wait for the effect coming from the left/right boundaries  
 427 of  $\Omega$  to propagate into the entire chain to reach a given tolerance. Hence, the “distributed”  
 428 homogeneous Dirichlet boundary condition in the two-dimensional case is the reason for the  
 429 scalability of the PSM, and this argument is also valid for the other domain decomposition  
 430 methods we discussed.

431 *Remark 1* If we have Neumann boundary conditions on the top and bottom boundaries of  
 432 the two dimensional problem, then PSM, OSM and PDNM do not scale, as one can see by  
 433 slightly adapting our analysis: the Neumann boundary condition implies the use of a cosine  
 434 Fourier series, instead of the sine Fourier series. The zero frequency is now included in  
 435 the expansion, i.e.  $e_j^n(x, y) = \sum_{m=0}^{\infty} v_j^n(x, k_m) \cos(k_m y)$ . For  $m = 0$ , the Fourier coefficient  $v_0^n$   
 436 satisfies the same equation as in the one dimensional case, and thus the scalability property  
 437 of the two dimensional case is lost due to the presence of this frequency, since the spectral  
 438 radius of the corresponding matrix deteriorates as the number of subdomains grows. For  
 439 the one level NNM the situation is even worse: NNM is not well posed then, since the sec-  
 440 ond step of the iteration would require the solution of pure Neumann problems for interior  
 441 subdomains, as in 1D.





**Fig. 16** Spectral radii of the iteration matrices for the different methods corresponding to  $L = 1/N$ ,  $\hat{L} = 1$ , and  $k = \pi$ . For PSM and OSM the overlap is rescaled as  $\delta = L/10$ .

442 *Remark 2* Our analysis can also be used to recover by a numerical evaluation of the con-  
 443 vergence factors the well-known results concerning the non scalability of one level domain  
 444 decomposition methods for fixed-size problems, where the subdomains become smaller and  
 445 smaller as their number grows, see for instance [40]: by setting  $L = 1/N$  and increasing the  
 446 number of subdomains, we see that the convergence factors of the classical and optimized  
 447 Schwarz methods and the Dirichlet-Neumann methods tend to 1 when the subdomain num-  
 448 ber increases, as shown in Figure 16. So these methods can not be weakly scalable in this  
 449 setting, in contrast to the case where the subdomain size remains fixed, as in the earlier sec-  
 450 tions. For the Neumann-Neumann method, the situation is even worse, since the assumption  
 451 of Theorem 6 is not satisfied anymore, and the method fails to converge when the number  
 452 of subdomains grows in this case.

453 *Remark 3* As an anonymous referee suggested, it is interesting to also consider the case of  
 454 a fixed number of multiple vertical layers of chains. In this case, the methods would still be  
 455 scalable when adding more and more subdomains in the horizontal direction, provided the  
 456 subdomain size remains fixed. This can be seen as follows: for a single layer of  $N$  subdo-  
 457 mains, we have seen that the contraction reaches the middle subdomain after  $\frac{N}{2}$  iterations.  
 458 To use this argument in the vertical direction, suppose for example that we have 5 vertical  
 459 layers: if we then consider 3 iterations, then the contraction given by the Dirichlet boundary  
 460 condition on the top and bottom reaches the middle layer, and thus all layers start contract-  
 461 ing. So looking in packets of 3 iterations, the errors will contract independently of how many  
 462 subdomains are added in the horizontal direction in each layer, due to our results for a single  
 463 layer.

## References

- 465 1. V. Barone and M. Cossi. Quantum calculation of molecular energies and energy gradients in solution by  
466 a conductor solvent model. *The Journal of Physical Chemistry A*, 102(11):1995–2001, 1998.
- 467 2. P. E. Björstad and O. B. Widlund. Iterative methods for the solution of elliptic problems on regions  
468 partitioned into substructures. *SIAM Journal on Numerical Analysis*, 23(6):1097–1120, 1986.
- 469 3. E. Cancès, Y. Maday, and B. Stamm. Domain decomposition for implicit solvation models. *The Journal*  
470 *of Chemical Physics*, 139:054111, 2013.
- 471 4. F. Chaouqui and M. J. Gander. Optimal coarse spaces for FETI and their approximation. *accepted in*  
472 *ENUMATH 2017 Proceedings*, 2018.
- 473 5. F. Chaouqui, M. J. Gander, and K. Santugini-Repique. On nilpotent subdomain iterations. In *Domain*  
474 *Decomposition Methods in Science and Engineering XXIII*, pages 125–133. Springer, Cham, 2017.
- 475 6. G. Ciaramella and M. J. Gander. Analysis of the parallel Schwarz method for growing chains of fixed-  
476 sized subdomains: Part I. *SIAM J. Num. Anal.*, 55(3):1330–1356, 2017.
- 477 7. G. Ciaramella and M. J. Gander. Analysis of the parallel Schwarz method for growing chains of fixed-  
478 sized subdomains: Part II. *SIAM J. Num. Anal.*, 56(3):1498–1524, 2018.
- 479 8. G. Ciaramella and M. J. Gander. Analysis of the parallel Schwarz method for growing chains of fixed-  
480 sized subdomains: Part III. *to appear in ETNA*, 2018.
- 481 9. V. Dolean, M. J. Gander, and L. Gerardo-Giorda. Optimized Schwarz methods for Maxwell’s equations.  
482 *SIAM Journal on Scientific Computing*, 31(3):2193–2213, 2009.
- 483 10. Maksymilian Dryja and Olof B. Widlund. *Multilevel additive methods for elliptic finite element prob-*  
484 *lems*. New York University, Department of Computer Science, Courant Institute of Mathematical Sci-  
485 ences, 1990.
- 486 11. O. Dubois, M. J. Gander, S. Loisel, A. St-Cyr, and D. B. Szyld. The optimized Schwarz method with a  
487 coarse grid correction. *SIAM Journal on Scientific Computing*, 34(1):A421–A458, 2012.
- 488 12. C. Farhat, M. Lesoinne, and K. Pierson. A scalable dual-primal domain decomposition method. *Numerical*  
489 *Linear Algebra with Applications*, 7(7-8):687–714, 2000.
- 490 13. M. J. Gander. Optimized Schwarz methods. *SIAM Journal on Numerical Analysis*, 44(2):699–731, 2006.
- 491 14. M. J. Gander. Schwarz methods over the course of time. *ETNA. Electronic Transactions on Numerical*  
492 *Analysis*, 31:228–255, 2008.
- 493 15. M. J. Gander and O. Dubois. Optimized Schwarz methods for a diffusion problem with discontinuous  
494 coefficient. *Numerical Algorithms*, 69(1):109–144, 2015.
- 495 16. M. J. Gander and L. Halpern. Méthodes de décomposition de domaine. *Encyclopédie électronique pour*  
496 *les ingénieurs*, 2012.
- 497 17. M. J. Gander, L. Halpern, and K. Santugini. Discontinuous coarse spaces for DD-methods with discon-  
498 tinuous iterates. In *Domain Decomposition Methods in Science and Engineering XXI*, pages 607–615.  
499 Springer, 2014.
- 500 18. M. J. Gander, L. Halpern, and K. Santugini. A new coarse grid correction for RAS/AS. In *Domain*  
501 *Decomposition Methods in Science and Engineering XXI*, pages 275–283. Springer, 2014.
- 502 19. M. J. Gander, L. Halpern, and K. Santugini. On optimal coarse spaces for domain decomposition and  
503 their approximation. In *Domain Decomposition Methods in Science and Engineering XXVI*. Springer,  
504 2018.
- 505 20. M. J. Gander and A. Loneland. *SHEM: An optimal coarse space for RAS and its multiscale approxima-*  
506 *tion*, pages 313–321. Springer International Publishing, Cham, 2017.
- 507 21. M. J. Gander, A. Loneland, and T. Rahman. Analysis of a new harmonically enriched multiscale coarse  
508 space for domain decomposition methods. *arXiv preprint arXiv:1512.05285*, 2015.
- 509 22. M. J. Gander, F. Magoules, and F. Nataf. Optimized Schwarz methods without overlap for the Helmholtz  
510 equation. *SIAM Journal on Scientific Computing*, 24(1):38–60, 2002.
- 511 23. M. J. Gander and M. Neumüller. Analysis of a new space-time parallel multigrid algorithm for parabolic  
512 problems. *SIAM Journal on Scientific Computing*, 38(4):A2173–A2208, 2016.
- 513 24. M. J. Gander and B. Song. Complete, optimal and optimized coarse spaces for Additive Schwarz. In  
514 *Domain Decomposition Methods in Science and Engineering XXVI*. Springer, 2017.
- 515 25. M. J. Gander and T. Vanzan. Heterogeneous optimized Schwarz methods for coupling Helmholtz and  
516 Laplace equations. *accepted in Domain Decomposition Methods in Science and Engineering XXIV*,  
517 2018.
- 518 26. M. J. Gander and T. Vanzan. Optimized Schwarz methods for advection diffusion equations in bounded  
519 domains. *accepted in ENUMATH 2017 Proceedings*, 2018.
- 520 27. Walter Gander, Martin J. Gander, and Felix Kwok. *Scientific computing-An introduction using Maple*  
521 *and MATLAB*, volume 11. Springer Science & Business, 2014.
- 522 28. C. Japhet, F. Nataf, and F. Rogier. The optimized order 2 method: application to convection–diffusion  
523 problems. *Future generation computer systems*, 18(1):17–30, 2001.

- 524 29. A. Klamt and G. Schuurmann. COSMO: a new approach to dielectric screening in solvents with explicit  
525 expressions for the screening energy and its gradient. *J. Chem. Soc., Perkin Trans. 2*, pages 799–805,  
526 1993.
- 527 30. Axel Klawonn and Oliver Rheinbach. Highly scalable parallel domain decomposition methods with  
528 an application to biomechanics. *ZAMM-Journal of Applied Mathematics and Mechanics/Zeitschrift für*  
529 *Angewandte Mathematik und Mechanik*, 90(1):5–32, 2010.
- 530 31. P.-L. Lions. On the Schwarz alternating method. I. *First international symposium on domain decompo-*  
531 *sition methods for partial differential equations*, pages 1–42, 1988.
- 532 32. P.-L. Lions. On the Schwarz alternating method. II. *Domain Decomposition Methods*, pages 47–70,  
533 1989.
- 534 33. P.-L. Lions. On the Schwarz alternating method. III: a variant for nonoverlapping subdomains. In *Third*  
535 *international symposium on domain decomposition methods for partial differential equations*, volume 6,  
536 pages 202–223. SIAM Philadelphia, PA, 1990.
- 537 34. F. Lipparini, G. Scalmani, L. Lagardère, B. Stamm, E. Cancès, Y. Maday, J.-P. Piquemal, M. J Frisch, and  
538 B. Mennucci. Quantum, classical, and hybrid QM/MM calculations in solution: General implementation  
539 of the ddCOSMO linear scaling strategy. *The Journal of chemical physics*, 141(18):184108, 2014.
- 540 35. F. Lipparini, B. Stamm, E. Cancès, Y. Maday, and B. Mennucci. Fast domain decomposition algorithm  
541 for continuum solvation models: Energy and first derivatives. *Journal of Chemical Theory and Computa-*  
542 *tion*, 9(8):3637–3648, 2013.
- 543 36. F. Nataf, F. Rogier, and E. de Sturler. *Optimal interface conditions for domain decomposition methods*.  
544 École polytechnique, 1994.
- 545 37. Roy A Nicolaides. Deflation of conjugate gradients with applications to boundary value problems. *SIAM*  
546 *Journal on Numerical Analysis*, 24(2):355–365, 1987.
- 547 38. A. Quarteroni and A. Valli. *Domain Decomposition Methods for Partial Differential Equations*. Numerical  
548 Mathematics and Scientific Computation. Clarendon Press, 1999.
- 549 39. Barry Smith, Petter Bjorstad, and William Gropp. *Domain decomposition: parallel multilevel methods*  
550 *for elliptic partial differential equations*. Cambridge university press, 2004.
- 551 40. A. Toselli and O. Widlund. *Domain Decomposition Methods: Algorithms and Theory*, volume 34.  
552 Springer, 2005.
- 553 41. T. N. Truong and E. V. Stefanovich. A new method for incorporating solvent effect into the classical, ab  
554 initio molecular orbital and density functional theory frameworks for arbitrary shape cavity. *Chemical*  
555 *Physics Letters*, 240(4):253–260, 1995.