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# HETEROGENEOUS OPTIMIZED SCHWARZ METHODS FOR SECOND ORDER ELLIPTIC PDES

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Abstract. Due to their property of convergence in the absence of overlap, optimized Schwarz 4 methods are the natural domain decomposition framework for heterogeneous problems, where the 5 spatial decomposition is provided by the multi-physics of the phenomena. We study here heteroge-6 7 neous problems which arise from the coupling of second order elliptic PDEs. Theoretical results and 8 asymptotic formulas are proposed solving the corresponding min-max problems both for single and 9 double sided optimizations, while numerical results confirm the effectiveness of our approach even when analytical conclusions are not available. Our analysis shows that optimized Schwarz methods 11 do not suffer the heterogeneity, it is the opposite, they are faster the stronger the heterogeneity is. It is even possible to have h independent convergence choosing two independent Robin parameters. 13 This property was proved for a Laplace equation with discontinuous coefficients, but only conjectured 14 for more general couplings in [12]. Our study is completed by an application to a contaminant transport problem. 15

16 **Key words.** Optimized Schwarz Methods - Heterogeneous Domain Decomposition Methods -17 Optimized Transmission Conditions - Contaminant Transport

### 18 **AMS subject classifications.** 65N55, 65N22, 65F10, 65F08

1. Introduction. The classical Schwarz method is a domain decomposition al-19 gorithm for solving large scale PDEs. It consists in dividing the domain of computa-20 tion into many subdomains, solving iteratively the local problems while exchanging information along the interfaces through Dirichlet boundary conditions. The pioneer-22 ing paper [25], in which Lions proposed a convergent algorithm using Robin transmis-23sion conditions, paved the way to the development of the optimized Schwarz methods 24 which exploit optimized transmission conditions in order to overcome some of the 2526 drawbacks of the classical Schwarz method such as slow convergence and overlap requirement [10]. The procedure to obtain such optimized transmission conditions is 27now well established [9]: the problem of interest is posed in a simplified setting where 28 one can use the Fourier transform, for unbounded domains, or Fourier series expansion 29 or more generally separation of variables [19, 18], for bounded domains, to transform 30 the PDE into a set of ODEs parametrized by the frequencies k. Then, solving the ODEs and using the transmission conditions, one can get a recursive relation for 32 the Fourier coefficients and obtain a closed formula for the convergence factor which contains some free parameters to optimize. 34

The literature regarding optimized Schwarz methods for homogeneous problems 35 is well developed. Optimized transmission conditions have been obtained for many 36 problems such as Helmholtz equations [16, 14], Maxwell equations [4, 22, 30], advec-37 tion diffusion problems [8, 18], Navier Stokes equations [3], shallow water equations 38 [27] and Euler equations [6]. In all the previous work, homogeneous problems are 39 analyzed, in the sense that a unique physics is considered in the whole domain, and 40 therefore the coupling on the interfaces regards equations of the same nature. First 41 attempts to generalize this situation have been carried out in [26], [12], where Laplace 42 equations with different diffusion coefficients were considered, and in [5], which was 43

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devoted to Maxwell equations with discontinuous coefficients. Let us remark that at 44 45least two possible interpretations of heterogeneous domain decomposition methods exist. The first one concerns problems where the same physical phenomenon is taking 46 place in the whole domain, but it can be convenient to use a cheaper approximation 47 in some parts of the domain in order to save computational resources. This might 48 be the case in the presence of boundary layers, or for example in CFD simulations 49 where a potential flow is used far away from the zone of interest while the Navier-50Stokes equations are fully solved near, for instance, an aircraft. In this situation, good 51transmission conditions can be obtained through a factorization approach, see [15] for further details. 53

In this manuscript we follow the second interpretation which assumes that two 5455different physical phenomena are present in the domain and they interact through an interface. In this case some physical coupling conditions must be satisfied along the 56 common interface, such as the continuity of the function and its normal derivative for second order PDEs, or the continuity of normal stresses for fluid-structure problems. 58 Some examples in this direction can be found in [17], where optimized transmission conditions were obtained for the coupling between the hard to solve Helmholtz equa-60 tion and the Laplace equation, or in [21] where a partial optimization procedure was 61 carried out for a fluid-structure problem. For this kind of heterogeneous problems, 62 a domain decomposition approach can be extremely useful since it allows to reuse 63 specific solvers designed for the different physics phenomena present in the domain. 64 For instance, one can use a finite volume solver where a strong advection is present 66 while using a multigrid solver where diffusion dominates or an ad-hoc linear elasticity solver combined with a CFD code for the Navier-Stokes equations. In this 67 perspective, optimized Schwarz methods lead to a significantly better convergence of 68 the coupling routine with respect to other domain decomposition algorithms (e.g. 69 Dirichlet-Neumann, Robin-Neumann) since they take into account the physical prop-70 erties in their transmission conditions. We refer the interested reader to [23, 24] for 7172 the application of optimized Schwarz methods for the coupling of atmospheric and oceanic computational simulation models. 73

We study here first the coupling between a reaction diffusion equation and a dif-74 fusion equation and second the harder coupling between a general second order PDE 75and a reaction diffusion equation. We provide theoretical results and asymptotic for-76 mulas for the optimized parameters, and we show the effectiveness through numerical 77 simulations. The manuscript is completed by the application of our results to a phys-78 ical model describing contaminant transport in underground media, which is a topic 79of great interest in the last thirty years due, for instance, to the increasing threat of 80 contamination of groundwater supplies by waste treatments and landfill sites or to 81 82 the disposal of nuclear radioactive waste [2]. We refer to [1] for a reference regarding modeling issues of contaminant transport. Our model assumes that the computa-83 tional domain  $\Omega = \Omega_1 \cup \Omega_2 \cup \Omega_3 \cup \Omega_4$ , represented in Figure 1, can be partitioned 84 into four layers. In the first one, the contaminant, whose concentration is described 85 through the unknown u, penetrates mainly thanks to rainfalls and therefore an ad-86 87 vection towards the negative y direction is present. The next two layers are formed by porous media so that the contaminant spreads in a diffusive regime described by 88 89 the Laplace equation. We furthermore suppose that in the second layer, some chemical reactions may take place which are synthesized in the reaction term. Finally in 90 the last layer, an underground flow transports the contaminant in the x direction to-91 wards a groundwater supply which is connected to a water well. The problem belongs 92 to the heterogeneous class, since in different parts of the domain we have different 93



Fig. 1: Geometry for the contaminant transport problem.

94 physical phenomena, and thus in the last paragraph we use the results discussed in 95 this manuscript to design an efficient domain decomposition method to compute the 96 stationary and time dependent distribution of the contaminant.

97 **2. Reaction Diffusion-Diffusion coupling.** Let us consider two domains  $\Omega_1 :=$ 98  $(-\infty, 0) \times (0, L)$  and  $\Omega_2 := (0, +\infty) \times (0, L)$  and the interface  $\Gamma := \{0\} \times (0, L)$ . In this 99 section we study a reaction-diffusion equation with discontinuous coefficients along the 100 interface  $\Gamma$ ,

101 (2.1) 
$$(\eta^2(x) - \nu(x)\Delta)u = f \quad \text{in} \quad \Omega,$$

where  $\Omega := \Omega_1 \cup \Omega_2$ ,  $\eta^2(x) = \eta^2 \ge 0$  in  $\Omega_1$  and  $\eta(x) = 0$  in  $\Omega_2$ , while  $\nu(x) = \nu_1$  in  $\Omega_1$  and  $\nu(x) = \nu_2$  in  $\Omega_2$ , with  $\nu_1, \nu_2 \in \mathbb{R}^+$ . Equation (2.1) is closed by homogeneous Dirichlet boundary conditions on the horizontal edges and assuming  $\lim_{x \to +\infty} u = 0$ .

105 The optimized Schwarz method for this problem is

$$(\eta^2 - \nu_1 \Delta) u_1^n = f \quad \text{in} \quad \Omega_1, \quad (\nu_1 \partial_x + S_1)(u_1^n)(0, \cdot) = (\nu_2 \partial_x + S_1)(u_2^{n-1})(0, \cdot), \\ -\nu_2 \Delta u_2^n = f \quad \text{in} \quad \Omega_2, \quad (\nu_2 \partial_x - S_2)(u_2^n)(0, \cdot) = (\nu_1 \partial_x - S_2)(u_1^{n-1})(0, \cdot),$$

107 where  $S_j$ , j = 1, 2 are linear operators along the interface  $\Gamma$  in the y direction. The 108 goal is to find which operators guarantee the best performance in terms of conver-109 gence speed. We consider the error equation whose unknowns are  $e_i^n := u_{|\Omega_i} - u_i^n$ , 100 i = 1, 2, and we expand the solutions in the Fourier basis in the y direction,  $e_i^n = \sum_{k \in \mathcal{V}} \hat{e}_i^n(x,k) \sin(ky), i = 1, 2$  with  $\mathcal{V} := \{\frac{\pi}{L}, \frac{2\pi}{L}, \ldots\}$ . Moreover we suppose that 112 the operator  $S_j$  are diagonalizable, with eigenvectors  $\psi_k(y) := \sin(ky)$ , such that 113  $S_j \psi_k = \sigma_j(k) \psi_k$ , where  $\sigma_j(k)$  are the eigenvalues of  $S_j$ . Under these assumptions, we 114 find that the coefficients  $\hat{e}_i^n$  satisfy,

$$(115 \quad (2.2) \quad \begin{aligned} &(\eta^2 - \nu_1 \partial_{xx} + \nu_1 k^2)(\hat{e}_1^n) &= 0, & k \in \mathcal{V}, \ x < 0, \\ &(\nu_1 \partial_x + \sigma_1(k))(\hat{e}_1^n)(0,k) &= (\nu_2 \partial_x + \sigma_1(k))(\hat{e}_2^{n-1})(0,k), & k \in \mathcal{V}, \\ &(-\nu_2 \partial_{xx} + \nu_2 k^2)(\hat{e}_2^n) &= 0, & k \in \mathcal{V}, \ x > 0, \\ &(\nu_2 \partial_x - \sigma_2(k))(\hat{e}_2^n)(0,k) &= (\nu_1 \partial_x - \sigma_2(k))(\hat{e}_1^{n-1})(0,k), & k \in \mathcal{V}. \end{aligned}$$

116 Solving the two differential equations parametrized by k in (2.2), imposing that the

solutions remain bounded for  $x \to \pm \infty$  and defining  $\lambda(k) := \sqrt{k^2 + \tilde{\eta}^2}$  and  $\gamma(k) := k$ ,

118 we obtain

119 (2.3) 
$$\hat{e}_1^n = \hat{e}_1^n(0,k)e^{\sqrt{k^2 + \bar{\eta}^2 x}} = \hat{e}_1^n(0,k)e^{\lambda(k)x} \quad \text{in} \quad \Omega_1, \\ \hat{e}_2^n = \hat{e}_2^n(0,k)e^{-kx} = \hat{e}_2^n(0,k)e^{-\gamma(k)x} \quad \text{in} \quad \Omega_2,$$

where  $\tilde{\eta}^2 = \frac{\eta^2}{\nu_1}$ . The transmission conditions in (2.2) allow us to express the Fourier coefficient at iteration n of the solution in one subdomain as function of the coefficient of the solution in the other subdomain at the previous iteration n-1, namely

123 (2.4) 
$$\hat{e}_1^n(0,k) = \frac{-\nu_2 \gamma(k) + \sigma_1(k)}{\nu_1 \lambda(k) + \sigma_1(k)} \hat{e}_2^{n-1}(0,k),$$

124 and

125 (2.5) 
$$\hat{e}_2^n(0,k) = \frac{\nu_1 \lambda(k) - \sigma_2(k)}{-\nu_2 \gamma(k) - \sigma_2(k)} \hat{e}_1^{n-1}(0,k).$$

126 Combining (2.4) and (2.5) we get

127 
$$\hat{e}_1^n(0,k) = \frac{-\nu_2\gamma(k) + \sigma_1(k)}{\nu_1\lambda(k) + \sigma_1(k)} \cdot \frac{\nu_1\lambda(k) - \sigma_2(k)}{-\nu_2\gamma(k) - \sigma_2(k)} \hat{e}_1^{n-2}(0,k).$$

128 By induction we then obtain

129 
$$\hat{e}_1^{2n}(0,k) = \rho^n \hat{e}_1^0(0,k)$$
  $\hat{e}_2^{2n}(0,k) = \rho^n \hat{e}_2^0(0,k),$ 

130 where the convergence factor  $\rho$  is defined by

131 
$$\rho := \rho(k, \sigma_1, \sigma_2) = \frac{-\nu_2 \gamma(k) + \sigma_1(k)}{\nu_1 \lambda(k) + \sigma_1(k)} \cdot \frac{\nu_1 \lambda(k) - \sigma_2(k)}{-\nu_2 \gamma(k) - \sigma_2(k)}$$

132 Expressing the dependence on the Fourier frequency k we get

133 (2.6) 
$$\rho(k,\sigma_1,\sigma_2) = \frac{-\nu_2 k + \sigma_1(k)}{\nu_1 \sqrt{k^2 + \tilde{\eta}^2} + \sigma_1(k)} \cdot \frac{\nu_1 \sqrt{k^2 + \tilde{\eta}^2} - \sigma_2(k)}{-\nu_2 k - \sigma_2(k)}.$$

134 A closer inspection of (2.6) leads us to conclude that if we chose the operators  $S_j$ 135 such that their eigenvalues are

136 (2.7) 
$$\sigma_1^{\text{opt}}(k) := \nu_2 k \text{ and } \sigma_2^{\text{opt}}(k) := \nu_1 \sqrt{k^2 + \tilde{\eta}^2},$$

then we would have  $\rho \equiv 0$ . In this case the algorithm would converge in just two 137iterations. This option, even tough it is optimal, leads to non local operators  $S_i^{\text{opt}}$ , 138 which correspond to the Schur complements [29], and they are expensive from the 139computational point of view. Indeed, the operator associated to the eigenvalues 140 $\sigma_1^{\text{opt}}(k) := \nu_2 k$  corresponds to the square root of the Laplacian on the interface  $\Gamma$ , i.e.  $S_1^{\text{opt}} = \nu_2(-\Delta_{\Gamma})^{\frac{1}{2}}$  which is a fractional and non local operator. The non-local property of  $S_1^{\text{opt}}$  can also be understood considering a discretization of the straight 141 142143interface  $\Gamma$  and the discrete counterpart of  $S_1^{\text{opt}}$ , i.e.  $S_{1h}^{\text{opt}} := \nu_2(-\Delta_{y,h})^{\frac{1}{2}}$  where  $-\Delta_{y,h} = \text{diag}(-1,2,-1)$  is the classical 1-D Laplacian. A direct implementation shows that the matrix  $S_{1h}^{\text{opt}}$  is dense. Even though the use of  $S_{1h}^{\text{opt}}$  would destroy the 144145146sparsity of the subdomain matrices, theoretically it could still be used as a transmis-147148sion condition and the method would then converge in two iterations. However, the

major drawback is that in general we do not know the operator  $S_j^{\text{opt}}$  and therefore we would have to assemble numerically the Schur complements. This is an operation which requires the knowledge of the inverse of the subdomain operators and therefore

152 it is computationally expensive.

We thus look for classes of convenient transmission conditions which are amenable 153to easy implementation, and then to find which transmission conditions among a 154specific class lead to the best convergence factor. We consider here zeroth order 155approximations of the optimal operators in (2.7) which correspond to classical Robin 156conditions on the interface. In order to get the best transmission conditions in terms 157of convergence speed, we have to minimize the maximum of the convergence factor 158over all the frequencies k. Defining  $\mathcal{D}_1, \mathcal{D}_2$  as the classes of transmission conditions, 159we are looking for a couple  $(\sigma_1^*, \sigma_2^*) \in \mathcal{D} := \mathcal{D}_1 \times \mathcal{D}_2$  such that 160

161 (2.8) 
$$(\sigma_1^*, \sigma_2^*) = \operatorname*{arg\,min}_{(\sigma_1, \sigma_2) \in \mathcal{D}} (\max_{k_{\min} \le k \le k_{\max}} |\rho(k, \sigma_1, \sigma_2)|).$$

162 The lower and upper bounds  $k_{\min}$ ,  $k_{\max}$  depend on the problem under study:  $k_{\min}$ 163 is given by the Fourier expansion and here it is equal to  $k_{\min} = \frac{\pi}{L}$ . The presence of 164  $k_{\min}$  in (2.8), is the "memory" that our problem has of the boundness of the domain, 165 see [11, 20, 19] for more details on the influence of the domain for optimized Schwarz 166 methods. The upper bound  $k_{\max}$  is instead the maximum frequency that can be 167 resolved by the grid and it is typically estimated as  $k_{\max} = \frac{\pi}{h}$  where h is a measure 168 of the grid spacing.

169 **2.1. Zeroth order single sided optimized transmission conditions.** Let *p* 170 be a free parameter, we define

171 (2.9) 
$$\sigma_1(k) = \nu_2 p, \quad \sigma_2(k) = \nu_1 \sqrt{\tilde{\eta}^2 + p^2}.$$

We have made this choice because the optimal operators in (2.7) are clearly 172rescaled according to the diffusion constants of the two subdomains and thus we 173imitate this behaviour. Furthermore we introduce the parameter  $\tilde{\eta}^2$  in the definition 174of  $\sigma_2(k)$  in order to make the problem amenable to analytical treatment. With this choice, we have  $\sigma_j(k) = \sigma_j^{opt}(k)$  for k = p; in other words, for the frequency k = p, 175176the transmission conditions lead to an exact solver which converges in two iterations. 177The idea of introducing free parameters such that the eigenvalues  $\sigma_i(k)$  are identical 178to the optimal ones for a certain frequency is essential, because as we will see in the 179180 following, it allows us to solve the min-max problems which, for a generic choice of  $\sigma_i$ , are extremely hard to solve. 181

Inserting the expressions (2.9) into (2.6), the min-max problem (2.8) becomes

183 (2.10) 
$$\min_{p \in \mathbb{R}} \max_{k_{\min} \le k \le k_{\max}} \left| \frac{k-p}{k+\lambda\sqrt{p^2+\tilde{\eta}^2}} \cdot \frac{\sqrt{k^2+\tilde{\eta}^2}-\sqrt{p^2+\tilde{\eta}^2}}{\sqrt{k^2+\tilde{\eta}^2}+\frac{p}{\lambda}} \right|,$$

184 where  $\lambda = \frac{\nu_1}{\nu_2}$ . We define  $\rho(k, p) := \frac{k-p}{k+\lambda\sqrt{p^2+\tilde{\eta}^2}} \cdot \frac{\sqrt{k^2+\tilde{\eta}^2}-\sqrt{p^2+\tilde{\eta}^2}}{\sqrt{k^2+\tilde{\eta}^2+\frac{p}{\lambda}}}$ . We are now solving 185 the min-max problem (2.10). The main steps are the following:

• Restricting the range in which we are searching for *p*.

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- Identifying the candidates for the maxima in the variable k.
- Studying how the maxima behave when varying the parameter p.

189 LEMMA 2.1 (Restriction for the interval of p). If  $p^*$  is a solution to problem 190 (2.10) then  $p^*$  belongs to the interval  $[k_{\min}, k_{\max}]$ . 191 Proof. First we note that  $|\rho(k,p)| < |\rho(k,-p)|$  for every  $p \ge 0$ . Therefore we can 192 assume  $p^* \in \mathbb{R}^+$ . Moreover the function is always positive and equal to zero only 193 for k = p. Thus we can neglect the absolute value. Direct calculations show that 194  $\frac{\partial \rho(k,p)}{\partial \mu} = h(k,p)$  where

222

195 
$$h(k,p) := \frac{(p-k)\lambda p(\sqrt{k^2 + \tilde{\eta}^2}\lambda + k)}{(k+\lambda\sqrt{p^2 + \tilde{\eta}^2})^2(\sqrt{k^2 + \tilde{\eta}^2}\lambda + p)\sqrt{p^2 + \tilde{\eta}^2}} + \frac{(\sqrt{p^2 + \tilde{\eta}^2} - \sqrt{k^2 + \tilde{\eta}^2})\lambda(\sqrt{k^2 + \tilde{\eta}^2}\lambda + k)}{(k+\lambda\sqrt{p^2 + \tilde{\eta}^2})(\sqrt{k^2 + \tilde{\eta}^2}\lambda + p)^2}.$$

We observe that if  $p^* < k_{\min}$  then  $\frac{\partial \rho}{\partial p}(k, p^*) < 0$  for all  $k \in [k_{\min}, k_{\max}]$ , hence we are for sure not at the optimum since increasing  $p^*$  would decrease the convergence factor for all the frequencies  $k \in [k_{\min}, k_{\max}]$ .

199 On the other hand if  $p^* > k_{\max}$  then we have  $\frac{\partial \rho}{\partial p}(k, p^*) > 0 \quad \forall k \in [k_{\min}, k_{\max}]$ . 200 Hence we cannot be at the optimum either since decreasing  $p^*$  would decrease  $\rho(k, p)$ 201  $\forall k \in [k_{\min}, k_{\max}]$ . Thus we can conclude that if  $p^*$  is a solution of (2.10), then  $p^*$  lies 202 in the interval  $[k_{\min}, k_{\max}]$ .

Now we focus on the search of the maxima of  $\rho(p, k)$  with respect to k keeping in mind that p belongs to  $[k_{\min}, k_{\max}]$ .

LEMMA 2.2 (Local maxima in k). For any fixed value of  $p \in [k_{\min}, k_{\max}]$ , the function  $k \to \rho(k, p)$  assumes its maximum either at  $k = k_{\min}$  or at  $k = k_{\max}$ .

207 Proof. We consider the derivative of  $\rho(k, p)$  with respect to k and we remind that 208  $\rho(k, p)$  is always positive so we may neglect the absolute value. Direct calculations 209 show that  $\frac{\partial \rho}{\partial k} = h(p, k)$ . Thus considering (2.11) we have that letting  $p \in (k_{\min}, k_{\max})$ , 210  $\frac{\partial \rho}{\partial k} < 0, \forall k < p$ , and  $\frac{\partial \rho}{\partial k} > 0, \forall k > p$ . Therefore the maximum is attained on the 211 boundary, either at  $k = k_{\min}$  or  $k = k_{\max}$ .

212 On the other hand, if  $p = k_{\min}$ ,  $\rho(k, k_{\min})$  has a zero in  $k = k_{\min}$ . For all the other 213 values of k in the interval  $[k_{\min}, k_{\max}]$ , the function is strictly increasing and therefore 214 the maximum is attained at  $k = k_{\max}$ . The case  $p = k_{\max}$  is identical and hence the 215 result follows.

We now have all the ingredients to solve the min-max problem (2.10).

THEOREM 2.3. The unique optimized Robin parameter  $p^*$  solving the min-max problem (2.10) is given by the unique root of the non linear equation

219 (2.12) 
$$|\rho(k_{\min}, p^*)| = |\rho(k_{\max}, p^*)|.$$

220 *Proof.* From the previous lemmas, we know that we can rewrite problem (2.10)221 as

$$\min_{p \in [k_{\min}, k_{\max}]} \max \left\{ \rho(k_{\min}, p), \rho(k_{\max}, p) \right\},\,$$

i.e. the maximum is either attained at  $k = k_{\min}$  or  $k = k_{\max}$ . We now show that the optimal  $p^*$  satisfies a classical equioscillation property [32], see Fig 2 for a graphical representation. We first note that  $\rho(k_{\min}, p) = 0$  for  $p = k_{\min}$ , and  $\frac{\partial \rho(k_{\min}, p)}{\partial p} > 0, \forall p \in$  $(k_{\min}, k_{\max}]$ . Therefore increasing p,  $\rho(k_{\min}, p)$  strictly increases until it reaches its maximum value for  $p = k_{\max}$ . On the other hand, we have that  $\rho(k_{\max}, k_{\min})$  is strictly greater than zero, and while p increases from  $k_{\min}$  to  $k_{\max}$ ,  $\rho(k_{\max}, p)$  decreases, being  $\frac{\partial \rho(k_{\max}, p)}{\partial p} < 0, \forall p \in [k_{\min}, k_{\max})$ . Furthermore we have that  $\rho(k_{\max}, k_{\max}) = 0$ .

Hence, thanks to the strict monotonicity of both  $\rho(k_{\min}, p)$  and  $\rho(k_{\max}, p)$ , there exists by continuity a unique value  $p^*$  such that  $\rho(k_{\min}, p^*) = \rho(k_{\max}, p^*)$ . This value is clearly the optimum, because perturbing  $p^*$  would increase the value of  $\rho$  at one of the two extrema and therefore the maximum of  $\rho$  over all k.



Fig. 2: Illustration of the equioscillation property described in Theorem 2.3.

Even though a closed form solution of (2.12) is not known, it is interesting to study asymptotically how the algorithm performs. Therefore we keep  $\nu_1$ ,  $\nu_2$  and  $\tilde{\eta}^2$  fixed, and  $k_{\max} = \frac{\pi}{h}$  while letting  $h \to 0$ . This is a case of interest since usually we want to decrease the mesh size h in order to get a better approximation and therefore it is useful to see how the method performs in this regime. We introduce the notation  $f(h) \sim g(h)$  as  $h \to 0$  if and only if  $\lim_{h\to 0} \frac{f(h)}{g(h)} = 1$ .

240 THEOREM 2.4. Let  $D := \sqrt{k_{\min}^2 + \tilde{\eta}^2}$ . Then if  $\nu_1, \nu_2, \tilde{\eta}^2$  are kept fixed,  $k_{\max} = \frac{\pi}{h}$ 241 and h is small enough, then the optimized Robin parameter  $p^*$  is given by

242 (2.13) 
$$p^* \sim C \cdot h^{-\frac{1}{2}}, \quad C := \sqrt{\frac{(\lambda D + k_{\min})\pi}{(\lambda + 1)}}.$$

Furthermore the asymptotic convergence factor of the heterogeneous optimized Schwarz
method is

245 (2.14) 
$$\max_{k_{\min} \le k \le \pi/h} |\rho(k, p^*)| \sim 1 - h^{\frac{1}{2}} \left[ \frac{\lambda D}{C} + \frac{D}{C} + \frac{k_{\min}}{\lambda C} + \frac{k_{\min}}{C} \right].$$

246 Proof. We make the ansatz  $p = C \cdot h^{-\alpha}$  in the equation (2.12). Expanding for 247 small h, we get that

248 
$$|\rho(k_{\min},p)| \sim 1 - h^{\alpha} \left[ \frac{\lambda D}{C} + \frac{D}{C} + \frac{k_{\min}}{\lambda C} + \frac{k_{\min}}{C} \right].$$

249 On the other hand,

250 
$$|\rho(k_{\max},p)| \sim 1 - h^{1-\alpha} \left[ \frac{\lambda C}{\pi} + \frac{2C}{\pi} + \frac{C}{\lambda \pi} \right].$$

251 Comparing the first two terms we get the result.

*Remark* 2.5. Note that if we set  $\tilde{\eta}^2 = 0$ , then we recover the results for the coupling of two Laplace equations with different diffusion constants, see [12]. In that case,

255 
$$\rho \sim 1 - h^{\frac{1}{2}} \sqrt{\frac{k_{\min}}{\pi}} \left[ \frac{(\lambda+1)^2}{\lambda} \right], \qquad p^* = \sqrt{k_{\min}\pi} h^{-\frac{1}{2}}.$$

$\tilde{\eta}$	$p^*$	$\bar{p}$	$\max_k \rho(k, p^*)$	$\max_k \rho(k, \bar{p})$
1	22.47	22.47	0.5618	0.5618
100	72.11	110.09	0.0737	0.0452
500	92.21	508.2691	0.0025	0.0081
1000	95	1005	$3.74 \cdot 10^{-4}$	0.0026

Table 1: Comparison between the optimal solution  $p^*$  of Theorem 2.3 and the optimal solution  $\bar{p}$  computed numerically for the min-max problem involving  $\sigma_1(k) = \nu_2 p$  and  $\sigma_2(k) = \nu_1 p$ . Mesh size equal to  $h = \frac{1}{50}$ .

Moreover we have that the convergence factor (2.14) satisfies for  $\lambda = \frac{\nu_1}{\nu_2} \to \infty$ ,  $|\rho| \sim 1 - h^{\frac{1}{2}} \lambda \sqrt{\frac{D}{\pi}}$  and for  $\lambda \to 0$ ,  $|\rho| \sim 1 - h^{\frac{1}{2}} \frac{1}{\lambda} \sqrt{\frac{k_{\min}}{\pi}}$ . On the other hand as  $\tilde{\eta} \to \infty$  we have  $|\rho| \sim 1 - h^{\frac{1}{2}} \sqrt{\tilde{\eta}} \frac{(\lambda+1)^{\frac{3}{2}}}{\sqrt{\lambda\pi}}$ . It follows that for all strong heterogeneity limits, the constant in front of the asymptotic term  $h^{\frac{1}{2}}$  becomes larger, therefore the deterioration is slower and the method is more efficient.

Remark 2.6. One could object that if we set  $\sigma_1(k) = \nu_2 p$  and  $\sigma_2(k) = \nu_1 p$ , with-261out introducing the ad-hoc term involving  $\tilde{\eta}$  in the definition  $\sigma_2(k)$ , it may be possible 262to improve the method. In this case the convergence factor would have two zeros, one 263located at  $k_1 := p$  and the other one located in  $k_2 := \sqrt{p^2 - \tilde{\eta}^2}$ . The min-max prob-264lem is then much harder to solve analytically because one of the zeros depends on 265the parameter p in a non-linear way. Furthermore for  $p < \tilde{\eta}$  the second zero is not 266real, for values of p slightly larger than  $\tilde{\eta}$ , the distance between the two zeros might 267be significant while if p is very large then  $k_1 \approx k_2$ . A large number of different cases 268arises which make the min-max problem really hard to solve. However, even tough 269we are unable to solve the min-max problem for a general setting of parameters, it is 270possible to draw conclusions in the case in which  $k_{\rm max}$  is large enough. In fact from 271an analysis of the convergence factor we deduce that  $\rho(k_{\max}, p) \to 1$  as  $h \to 0$ . If we 272impose equioscillation between  $\rho(k_{\min}, p)$  and  $\rho(k_{\max}, p)$ , calculations show that then 273p goes to infinity as  $h \to 0$  and therefore we have three local maxima in the interval 274 $[k_{\min}, k_{\max}]$ , two at the boundary and an interior maximum, k located between the 275two zeros. Estimating asymptotically  $|\rho(\hat{k},p)|$  as  $h \to 0$  using the convexity of the 276function in the interval  $[k_1, k_2]$  we obtain 277

278 
$$|\rho(\hat{k},p)| \le \frac{\partial \rho}{\partial k}|_{(k=\sqrt{p^2-\tilde{\eta}^2},p)} \cdot |p-\sqrt{p^2-\tilde{\eta}^2}| \approx h^2 + o(h^2).$$

Then observing instead that the value of  $\rho$  tends to one at the boundaries, it follows 279that the optimal solution is indeed obtained by equioscillations between the extreme 280 points and the interior point does not play a role. Repeating the analogous calculations 281of Theorem 2.4, we find that p has the same asymptotic expression as in the previous 282 theorem. We can then conclude that, for  $h \to 0$ , the two min-max problems with 283different  $\sigma_2(k)$  lead to equivalent optimized parameters. In the non asymptotic regime, 284Table 1 shows that the two choices are equivalent for moderate values of  $\tilde{\eta}$ . For very 285large values of  $\tilde{\eta}$ , then (2.9) leads to a more efficient method. 286

**2.2. Zeroth order two sided optimized transmission conditions.** Let us consider now the more general case for Robin transmission conditions, with two free

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289 parameters p and q such that the operators  $S_j$  have eigenvalues

290 
$$\sigma_1(k) = \nu_2 p, \quad \sigma_2(k) = \nu_1 \sqrt{q^2 + \tilde{\eta}^2}$$

291 We remark that, according to this choice,  $\sigma_1(k)$  is exact for the frequency k = p

while  $\sigma_2(k)$  is exact for frequency k = q. Therefore from (2.6) we deduce the method converges in two iterations for two frequencies. Letting again  $\lambda = \frac{\nu_1}{\nu_2}$ , we get (2.15)

294 
$$\min_{p,q} \max_{k_{\min} \le k \le k_{\max}} |\rho(k,p,q)| = \min_{p,q} \max_{k_{\min} \le k \le k_{\max}} \left| \frac{(k-p)(\sqrt{k^2 + \tilde{\eta}^2} - \sqrt{q^2 + \tilde{\eta}^2})}{(k + \lambda\sqrt{q^2 + \tilde{\eta}^2})(\sqrt{k^2 + \tilde{\eta}^2 + \frac{p}{\lambda}})} \right|.$$

Following the same philosophy of the previous section, we start restricting the range in which we need to search for the parameters p and q. Then we focus on the maxima with respect to k and finally we analyse how these maxima behave with respect to pand q.

LEMMA 2.7 (Restriction for the interval of p, q). If the couple  $(p^*, q^*)$  is a solution to the min-max problem (2.15), then we have that both  $p^*$  and  $q^*$  belong to the interval  $[k_{\min}, k_{\max}]$ .

302 *Proof.* For p > 0, we observe that  $|\rho(k, p, q|) < |\rho(k, -p, q)|$  and q is always 303 squared so we can restrict both parameters to be positive without loss of generality. 304 Next we consider the partial derivatives of  $|\rho|$  with respect to p and q:

305 (2.16) 
$$\operatorname{sign}\left(\frac{\partial|\rho|}{\partial p}\right) = -\operatorname{sign}(k-p), \quad \operatorname{sign}\left(\frac{\partial|\rho|}{\partial q}\right) = -\operatorname{sign}(k-q).$$

Repeating the same argument of Lemma 2.1, we conclude that we are not at the optimum unless both p and q belong to  $[k_{\min}, k_{\max}]$ .

Next we analyse the behaviour of  $|\rho(k, p, q)|$  with respect to the variable k, trying to identify the local maxima.

310 LEMMA 2.8 (Local maxima in k). For  $p, q \in [k_{\min}, k_{\max}]$ ,

311 
$$\max_{k_{\min} \le k \le k_{\max}} |\rho(k, p, q)| = \max\{|\rho(k_{\min}, p, q)|, |\rho(k, p, q)|, |\rho(k_{\max}, p, q)|\},\$$

312 where  $\hat{k}$  is an interior maximum always between  $[\min(p,q), \max(p,q)]$ .

Proof. We first observe that  $|\rho(k, p, q)|$  has two zeros, one at k = p and the other at k = q. Next we consider the derivative of  $\rho(k, p, q)$  with respect to k and assuming that  $p \neq q^1$  we get,

$$(2.17) \qquad \frac{\partial \rho(k,p,q)}{\partial k} = \frac{(\sqrt{k^2 + \tilde{\eta}^2} - \sqrt{q^2 + \tilde{\eta}^2})(\sqrt{k^2 + \tilde{\eta}^2})(\sqrt{k^2 + \tilde{\eta}^2} + \frac{p}{\lambda})(\lambda\sqrt{q^2 + \tilde{\eta}^2} + p)}{D(k,p)} + \frac{(k-p)(k + \lambda\sqrt{q^2 + \tilde{\eta}^2})k(\frac{p}{\lambda} + \sqrt{q^2 + \tilde{\eta}^2})}{D(k,p)}.$$

317 The denominator D(k, p) is always positive. Now we consider the two cases in which

318  $k < \min(p,q)$  and  $k > \max(p,q)$ : in both we have that  $\rho(k,p,q) > 0$ , and analyzing 319 equation (2.17) we conclude that for  $k < \min(p,q)$ ,  $\frac{\partial \rho(k,p)}{\partial k} < 0$  and for  $k > \max(p,q)$ ,

equation (2.17) we conclude that for  $k < \min(p,q)$ ,  $\frac{-\partial k}{\partial k} < 0$  and for  $k > \max(p,q)$ 

<sup>&</sup>lt;sup>1</sup>If p = q we are considering the optimization problem discussed in the previous paragraph.



Fig. 3: The left panel shows an example of the convergence factor with its three local maxima localized at  $k = k_{\min}$ ,  $k = k_{\max}$  and  $k = \tilde{k}$ . On the right we summarizes how these local maxima behave as function of p and q.

<sup>320</sup>  $\frac{\partial \rho}{\partial k} > 0$ . Hence by continuity of  $\partial_k \rho(k, p)$ , there exits at least one  $\hat{k}$ , which is a local <sup>321</sup> minimum of  $\rho(k, p)$  and a local maximum for  $|\rho(k, p)|$  see Fig. 3, such that  $\partial_k \rho = 0$ , <sup>322</sup> and all of them lie in the interval  $[\min(p, q), \max(p, q)]$  for p and q fixed. Now we <sup>323</sup> prove that the interior maximum is unique. Indeed the interior maxima for  $|\rho(k, p, q)|$ <sup>324</sup> are given by the roots of the equation  $\partial_k \rho(k, p) = 0$  which corresponds to

325 (2.18) 
$$\frac{\sqrt{q^2 + \tilde{\eta}^2} - \sqrt{\tilde{\eta}^2 + k^2}}{k + \lambda \sqrt{\tilde{\eta}^2 + q^2}} = \frac{(k-p)k}{\left(\lambda \sqrt{k^2 + \tilde{\eta}^2} + p\right)\sqrt{k^2 + \tilde{\eta}^2}}.$$

First we suppose that p < k < q. Then we have that the left hand side of (2.18) is positive in k = p, it is strictly decreasing in k, and it reaches zero at k = q. The right hand side of (2.18) instead starts from zero and it is strictly increasing. We conclude that there is a unique point  $\hat{k}$  such that the two sides are equal and hence a unique interior maximum  $\hat{k}$  for  $|\rho(k, p, q)|$ . If instead q < k < p, changing the sign of (2.18) and diving by  $k/\sqrt{k^2 + \tilde{\eta}^2}$ , the right hand side is strictly decreasing while the left hand side, computing the derivative, is strictly increasing and hence the same conclusion holds.

We may conclude that the function assumes its maximum either at the interior point  $\hat{k}$ , or at the boundaries of the interval, i.e.  $k_{\min}$ ,  $k_{\max}$ .

In the next lemma we prove that the end points  $k_{\min}$  and  $k_{\max}$  satisfy an equioscillation property as in the previous case of a single parameter p.

LEMMA 2.9 (Equioscillation at the end points). The optimized convergence factor  $|\rho(k, p, q)|$  must satisfy equioscillation at the endpoints, i.e.

340 
$$|\rho(k_{\min}, p^*, q^*)| = |\rho(k_{\max}, p^*, q^*)|.$$

341 *Proof.* We study how  $|\rho(k_{\min}, p, q)|$ ,  $|\rho(\tilde{k}, p, q)|$  and  $|\rho(k_{\max}, p, q)|$  behave as p, q342 vary and we show that if we do not have equioscillation at the boundary points, we 343 can always improve the convergence factor until equioscillation is reached. Taking 344 into account (2.16) we have for every  $p, q \in [k_{\min}, k_{\max}]$ 

345 
$$\frac{\partial |\rho(k_{\min}, p, q)|}{\partial p} > 0, \quad \frac{\partial |\rho(k_{\min}, p, q)|}{\partial q} > 0$$

346347

$$rac{\partial |
ho(k_{\max},p,q)|}{\partial p} < 0, \quad rac{\partial |
ho(k_{\max},p,q)|}{\partial q} < 0$$

In other words, increasing independently p, q increases  $|\rho(k_{\min}, p, q)|$  and decreases  $|\rho(k_{\max}, p, q)|$ . We now compute the total derivative of  $|\rho(\tilde{k}, p, q)|$  with respect to pand q, which since we have  $\partial_k |\rho(\tilde{k}, p, q)| = 0$ , corresponds to the partial derivative with respect to the two arguments. One then finds that the sign of  $\frac{\partial |\rho(\tilde{k}, p, q)|}{\partial p}$  and  $\frac{\partial |\rho(\tilde{k}, p, q)|}{\partial q}$  depends on the position of  $\tilde{k}$  with respect to p and q. Indeed it holds

353 
$$\operatorname{sign}\left(\frac{\partial|\rho(\tilde{k}, p, q)|}{\partial p}\right) = \operatorname{sign}(p - \tilde{k}), \quad \operatorname{sign}\left(\frac{\partial|\rho(\tilde{k}, p, q)|}{\partial q}\right) = \operatorname{sign}(q - \tilde{k})$$

354The right panel of Fig. 3 summarizes the dependence of the local maxima with respect to p and q. Let us suppose that p < q, q fixed, and  $|\rho(k_{\min}, p, q)| < |\rho(k_{\max}, p, q)|$ . 355 The other cases are treated similarly. We do not make any assumptions on the value of 356  $|\rho(\hat{k}, p, q)|$ . Now if we increase p we decrease max{ $|\rho(k_{\min}, p, q)|, |\rho(\hat{k}, p, q)|, |\rho(k_{\max}, p, q)|$ } 357 as long as  $|\rho(k_{\min}, p, q)| \leq |\rho(k_{\max}, p, q)|$  and  $p \leq q$ . If  $|\rho(k_{\min}, p, q)| = |\rho(k_{\max}, p, q)|$ 358 for a certain p < q, then we obtain the desired result since we have improved 359uniformly the convergence factor. Suppose instead that when p = q, and there-360 fore  $|\rho(k, p, q)| = 0$ , we still have  $|\rho(k_{\min}, p, q)| < |\rho(k_{\max}, p, q)|$ . Thus the conver-361 gence factor is equal to  $|\rho(k_{\max}, p, q)|$ . We now set up a process which improves 362  $\max_{[k_{\min},k_{\max}]} |\rho(k,p,q)|$  until we get equioscillation at the boundary points. As long 363 as  $|\rho(k_{\min}, p, q)| < |\rho(k_{\max}, p, q)|$ , we increase p > q until  $|\rho(k, p, q)| \le |\rho(k_{\max}, p, q)|$ . 364 When we reach  $|\rho(k, p, q)| = |\rho(k_{\max}, p, q)|$ , we then increase q until q = p. If while 365 increasing q we still have  $|\rho(k_{\min}, p, q)| < |\rho(k_{\max}, p, q)|$ , then we repeat the process. 366 Continuing this process, we must reach equioscillation at some point by continuity 367 368 since when p approaches  $k_{\max}$ , we must have  $|\rho(k_{\min}, k_{\max}, q)| > |\rho(k_{\max}, k_{\max}, q)| = 0$ . At the same time we improved surely the convergence factor since, in spite of the ini-369 tial value of  $|\rho(k, p, q)|$ , we have that  $\max_{[k_{\min}, k_{\max}]} |\rho(k, p, q)| \leq |\rho(k_{\max}, p, q)|$  which 370 is decreasing along the process. Π 371

372 We now have enough tools and insights to prove the main results of this section:

THEOREM 2.10. There are two pairs of parameters  $(p_1^*, q_1^*)$  and  $(p_2^*, q_2^*)$  such that we obtain equioscillation between all the three local maxima,

375 (2.19) 
$$|\rho(k_{\min}, p_j^*, q_j^*)| = |\rho(k_{\max}, p_j^*, q_j^*)| = |\rho(k, p_j^*, q_j^*)| \quad j = 1, 2.$$

376 The optimal pair of parameters is the one which realizes the

377 (2.20) 
$$\min_{(p_j^*, q_j^*), j=1,2} |\rho(k_{\min}, p_j^*, q_j^*)|.$$

*Proof.* Let us define  $F_1(p,q) := \rho(k_{\min}, p, q)$  and  $F_2(p,q) := \rho(k_{\max}, p, q)$ . Due to Lemma 2.9, we know that there exist values (p,q) such that  $F := |F_1(p,q)| - |F_2(p,q)| = 0$ . We can thus express one parameter, for example q, as a function of the other one, i.e. q = q(p). Although the expression is too complicated to be used for analytical computations, we are able to infer about the structure of q(p). First of all we can state that  $q(p = k_{\min}) = k_{\max}$  since  $|F_1(k_{\min}, q(k_{\min}))| = 0$  implies that  $|F_2(k_{\min}, q(k_{\min})| = 0$  but then the only choice possible is  $q(k_{\min}) = k_{\max}$ . Similarly we have  $q(k_{\max}) = k_{\min}$ . We next use implicit differentiation to infer about the

behaviour of q with respect to p.

Following classical arguments we have that, since F(p, q(p)) = 0,

$$0 = \frac{dF(p,q(p))}{dp} = \frac{dF_1(p,q(p)) - dF_2(p,q(p))}{dp} = \frac{\partial F_1 - \partial F_2}{\partial p} + \frac{\partial F_1 - \partial F_2}{\partial q}q'(p)$$

and therefore 378

379 (2.21) 
$$q'(p) = \frac{\frac{\partial F_2}{\partial p} - \frac{\partial F_1}{\partial p}}{\frac{\partial F_1}{\partial q} - \frac{\partial F_2}{\partial q}}.$$

Analyzing carefully the sign of each term, we conclude that  $q'(p) < 0 \quad \forall p \in (k_{\min}, k_{\max}).$ 380 Therefore we state that q(p) is a strictly decreasing function which starts from q(p)381  $k_{\min}$  =  $k_{\max}$  and reaches its minimum at  $q(k_{\max}) = k_{\min}$ . 382

383 Now we have only one free parameter p, since q is constrained to vary such that the equioscillation between the ends points is achieved, thus we look for values of p such 384that we obtain equioscillation between  $k_{\min}$  and the interior maximum k. 385

Let us first study how  $\tilde{F}(p,q) := \rho(\hat{k}, p, q(p))$  behaves while p varies. As long as 386 $p \leq \hat{k} \leq q(p)$ , we have 387

Then, keeping in mind the q'(p) < 0,  $\tilde{F}(p,q(p))$  is strictly decreasing for all the values 391 of p such that  $p < \hat{k} < q(p)$ , 392

$$\frac{d|F(p,q(p))|}{dp} = \frac{\partial|F(p,q(p))|}{\partial p} + \frac{\partial|F(p,q(p))|}{\partial q} \cdot q'(p) < 0.$$

Similarly it is straightforward to verify that for  $q(p) < \hat{k} < p$ 394

395 
$$\frac{d|\tilde{F}(p,q(p))|}{dp} = \frac{\partial|\tilde{F}(p,q(p))|}{\partial p} + \frac{\partial|\tilde{F}(p,q(p))|}{\partial q} \cdot q'(p) > 0.$$

Moreover we have that for  $p = \hat{k} = q(p), |\tilde{F}(p,q(p))| = 0$  and  $\frac{d|\tilde{F}(p,q(p))|}{dp} = 0.$ 396

Focusing next on  $|F_1(p,q(p))|$  we can state that, neglecting the sign $(F_1(p,q(p)))$ , be-397 398 cause it is always positive or zero, the derivatives at the left and right boundary extrema are equal to 399

$$400 \quad \frac{d|F_1(k_{\min},k_{\max})|}{dp} = \frac{\partial|F_1(k_{\min},k_{\max})|}{\partial p} + \frac{\partial|F_1(k_{\min},k_{\max})|}{\partial q}q'(p) = \frac{\partial|F_1(k_{\min},k_{\max})|}{\partial p} > 0,$$

and 401

$$402 \quad \frac{d|F_1(k_{\max},k_{\min})|}{dp} = \frac{\partial|F_1(k_{\max},k_{\min})|}{\partial p} + \frac{\partial|F_1(k_{\max},k_{\min})|}{\partial q}q'(p) = \frac{\partial|F_1(k_{\max},k_{\min})|}{\partial p} < 0.$$

So for values of p in a right neighbourhood of  $p = k_{\min}$ ,  $|F_1(p, q(p))|$  increases, while 403404 for values of p in a left neighbourhood of  $p = k_{\max}$ ,  $|F_1(p, q(p))|$  decreases. Using the

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monotonicity of  $|F(\hat{k}, p, q(p))|$  and the fact that when  $\hat{k} = p = q(p), |F(\hat{k}, p, q(p))| = 0$ , while  $|F(k_{\min}, p, q(p))| > 0$ , we conclude that there exists at least one pair (p, q) such that  $|F(k_{\min}, p, q(p))| = |F(\hat{k}, p, q(p))|$ .

We still have to prove that actually there exist only two couples  $(p_j, q_j)$  such that equioscillation is achieved. Indeed, if we imagine that  $|F_1(p, q(p))|$  had a certain behaviour, for example it oscillates, then we might have more than two pairs. Nevertheless we show that  $|F_1(p, q(p))|$  has a unique local maximum for  $p \in [k_{\min}, k_{\max}]$ so that only two equioscillations are allowed among all the three local maxima: one while  $|\tilde{F}(p, q(p))|$  decreases, the other one for increasing  $|\tilde{F}(p, q(p))|$ .

414 To do so, we consider  $\frac{d|F_1(p,q(p))|}{dp}$  again and substitute (2.21),

415 
$$\frac{d|F_1(p,q(p))|}{dp} = \frac{\frac{\partial F_1}{\partial q} \cdot \frac{\partial F_2}{\partial p} - \frac{\partial F_2}{\partial q} \cdot \frac{\partial F_1}{\partial p}}{\frac{\partial F_1}{\partial q} \cdot \frac{\partial F_2}{\partial q}}$$

416 The zeros of the derivative are given by the non linear equation

417 
$$(p - k_{\min})(\sqrt{k_{\max}^2 + \tilde{\eta}^2} - \sqrt{k_{\min}^2 + \tilde{\eta}^2}) \frac{\sqrt{k_{\min}^2 + \tilde{\eta}^2 + \frac{p}{\lambda}}}{\sqrt{k_{\max}^2 + \tilde{\eta}^2 + \frac{p}{\lambda}}}$$

418  
419  
(
$$k_{\max} - p$$
) $(\sqrt{q^2 + \tilde{\eta}^2} - \sqrt{k_{\min}^2 + \tilde{\eta}^2}) \frac{k_{\min} + \lambda \sqrt{q^2 + \tilde{\eta}^2}}{k_{\max} + \lambda \sqrt{q^2 + \tilde{\eta}^2}}$ 

It is sufficient to observe that the left hand side starts from 0 and it is strictly increasing 420 in p, while the right hand side starts from a positive value, it decreases with p and 421it reaches 0 for  $p = k_{\text{max}}$ . So the equation admits only one solution and therefore 422 the local maximum with respect to p of  $|F_1(p,q(p))|$  is unique. The solution to the 423 min-max problem (2.15) is the pair of parameters  $(p^*, q^*)$  which allows equioscillation 424 among the three local maxima and realizes (2.20). Every other pair of parameter 425 426 would led to the increase of at least one of the local maxima and therefore of the maximum of  $|\rho|$  over k. 427

428 In [12], the authors proved a similar result for the Laplace equation with discontinuous coefficients without the presence of the further optimality condition (2.20). 429 Their result was based on the possibility to restrict the interval of interest for the pa-430rameters to p < q or q < p according to the value of  $\lambda$ . In the present case this is not 431 possible because of the presence of  $\tilde{\eta}^2$  which breaks the symmetry of the convergence 432 433 factor. Therefore we cannot discard a priori one of the two possible equioscillations and the further condition (2.20) must be added. Nevertheless in the asymptotic regime 434 for  $h \to 0$  and  $k_{\rm max} \to \infty$ , the next result allows us to clearly choose the optimal pair 435 as a function of  $\lambda$ , recovering the property of the results for the simplified situation 436 treated in [12]. 437

438 THEOREM 2.11. Let  $D := \sqrt{k_{\min}^2 + \tilde{\eta}^2}$ . Then if the physical parameters  $\tilde{\eta}^2, \nu_1, \nu_2$ 439 are fixed,  $k_{\max} = \frac{\pi}{h}$  and h goes to zero, the optimized two-sided Robin parameters are 440 for  $\lambda \geq 1$ ,

441 (2.22) 
$$p_{1}^{*} \sim \frac{\lambda(k_{\min}+D)}{\lambda-1} - \frac{2\sqrt{2}(1+\lambda)(\lambda D + k_{\min})\lambda^{2}\sqrt{\pi(k_{\min}+D)}}{\pi\lambda(\lambda-1)^{3}}h^{\frac{1}{2}},$$
  

$$q_{1}^{*} \sim \frac{\pi(\lambda-1)}{2\lambda}h^{-1} + \frac{\sqrt{2}(1+\lambda)^{2}\sqrt{\pi(k_{\min}+D)}}{2\lambda(\lambda-1)}h^{-\frac{1}{2}},$$
  

$$\max_{k_{\min}\leq k\leq \pi/h}|\rho(k,p_{1}^{*},q_{1}^{*})| \sim \frac{1}{\lambda} - \frac{2\sqrt{2}(1+\lambda)\sqrt{(k_{\min}+D)}}{\sqrt{\pi\lambda(\lambda-1)}}h^{\frac{1}{2}},$$

442 and for  $\lambda < 1$  we have

$$p_{2}^{*} \sim \frac{1}{2}\pi(1-\lambda)h^{-1} + \frac{\sqrt{2}(1+\lambda)^{2}\sqrt{\pi(D+k_{\min})}}{2(1-\lambda)}h^{-\frac{1}{2}},$$

$$q_{2}^{*} \sim \sqrt{\left(\frac{D+k_{\min}}{1-\lambda}\right)^{2} - \tilde{\eta}^{2}} - \frac{2\sqrt{2}(D+k_{\min})^{2}(\lambda+1)(\lambda D+k_{\min})}{(\lambda-1)^{4}\sqrt{\pi(D+k_{\min})}\sqrt{\frac{D+k_{\min}}{1-\lambda} - \tilde{\eta}^{2}}}h^{\frac{1}{2}},$$

$$\max_{k_{\min} \leq k \leq \pi/h} |\rho(k, p_{2}^{*}, q_{2}^{*})| \sim \lambda - \frac{2\sqrt{2}\lambda(1+\lambda)\sqrt{(k_{\min}+D)}}{\sqrt{\pi(1-\lambda)}}h^{\frac{1}{2}}.$$

444 Proof. Guided by numerical experiments, for  $\lambda \geq 1$  we make the ansatz  $p \sim C_p + Ah^{\frac{1}{2}}$ ,  $q \sim Qh^{-1} + Bh^{-\frac{1}{2}}$ , and  $\hat{k} = C_k h^{-\frac{1}{2}}$ . First of all considering the equation 445  $\partial_k \rho(\hat{k}, p, q) = 0$ , we find setting to zero the first non zero term  $C_k = \sqrt{C_p \cdot Q}$ . Insert-447 ing this into (2.19) and comparing the two leading terms, we get the result. Similarly 448 for  $\lambda < 1$ , we make the ansatz  $p \sim C_p h^{-1} + Ah^{-\frac{1}{2}}$ ,  $q \sim Q + Bh^{\frac{1}{2}}$  and  $\hat{k} = C_k h^{-\frac{1}{2}}$  and 449 we get  $C_k = \sqrt{C_p \sqrt{Q^2 + \tilde{\eta}^2}}$ . Substituting and matching the leading order terms we 450 obtain the result.

If we set  $\tilde{\eta}^2 = 0$ , then  $D = k_{\min}$  and we recover the results of [12]. Note that in 451 contrast to the one sided case, the convergence factor does not deteriorate to 1 as 452 $h \to 0$ , but it is bounded either by  $\frac{1}{\lambda}$  if  $\lambda \geq 1$  or by  $\lambda$  if  $\lambda < 1$ , so we obtain a non-453overlapping optimized Schwarz method that converges independently of the mesh size 454h. We emphasize that the heterogeneity makes the method faster instead of presenting 455a difficulty. A heuristic explanation is that the heterogeneity tends to decouple the 456 problems, making them less dependent one from the other. In contrast with other 457domain decomposition methods, optimized Schwarz methods can be tuned according 458to the physics and therefore they can benefit from this decoupling. 459

**3.** Advection Reaction Diffusion-Reaction Diffusion coupling. In this section, we consider again a domain  $\Omega$  divided into two subdomains,  $\Omega_1, \Omega_2$  according to the description at the beginning of Section 2. In  $\Omega_1$  we have a reaction diffusion equation, while in  $\Omega_2$  we have an advection reaction diffusion equation. We allow the reaction and diffusion coefficients to be different among the subdomains. The optimized Schwarz method reads

$$\begin{array}{rcl} (\eta_1^2 - \nu_1 \Delta) u_1^n &= f, & \text{in} \quad \Omega_1, \\ (\nu_1 \partial_x + S_1)(u_1^n)(0, \cdot) &= (\nu_2 \partial_x - \mathbf{a} \cdot (1, 0)^\top + S_1)(u_2^{n-1})(0, \cdot), \\ (\eta_2^2 + \mathbf{a} \cdot \nabla - \nu_2 \Delta) u_2^n &= f, & \text{in} \quad \Omega_2, \\ (\nu_2 \partial_x - \mathbf{a} \cdot (1, 0)^\top - S_2)(u_2^n)(0, \cdot) &= (\nu_1 \partial_x - S_2)(u_1^{n-1})(0, \cdot), \end{array}$$

467 where  $\mathbf{a} = (a_1, a_2)^{\top}$ . The additional term in the transmission conditions arises from 468 the conservation of the flux in divergence form, see Chapter 6 in [31]. We first suppose 469  $a_2 = 0$ . Then we can solve the error equations in the subdomains through separation 470 of variables and we obtain  $e_i^n = \sum_{k \in \mathcal{V}} \hat{e}_i^n \sin(ky), i = 1, 2$ , where

471 
$$\hat{e}_1^n(k,x) = A^n(k)e^{\sqrt{\frac{\eta_1^2}{\nu_1} + k^2}x} \qquad \hat{e}_2^n(k,x) = B^n(k)e^{\lambda_-(k)x},$$

and  $\lambda_{-}(k) := \frac{a_1 - \sqrt{a_1^2 + 4\nu_2^2 k^2 + 4\nu_2 \eta_2^2}}{2\nu_2}$ . Inserting  $e_1, e_2$  into the transmission conditions 472 473 we get

$$\nu_1 \sqrt{\frac{\eta_1^2}{\nu_1} + k^2 A^n(k) + \sigma_1(k) A^n(k)} = \nu_2 \lambda_-(k) B^{n-1}(k) - a_1 B^{n-1}(k) + \sigma_1(k) B^{n-1}(k),$$

$$\nu_2 \lambda_-(k) B^n(k) - a_1 B^n(k) - \sigma_2(k) B^n(k) = \nu_1 \sqrt{\frac{\eta_1^2}{\nu_1}} + k^2 A^{n-1}(k) - \sigma_2(k) A^{n-1}(k)$$

The convergence factor is therefore given by 475

476 
$$\rho(k,\sigma_1,\sigma_2) = \frac{\nu_2 \lambda_-(k) - a_1 + \sigma_1(k)}{\nu_1 \sqrt{\tilde{\eta}_1^2 + k^2} + \sigma_1(k)} \frac{\nu_1 \sqrt{\tilde{\eta}_1^2 + k^2} - \sigma_2(k)}{\nu_2 \lambda_-(k) - a_1 - \sigma_2(k)},$$

where  $\tilde{\eta}_1^2 = \frac{\eta_1^2}{\nu_1}$ . We rewrite  $\lambda_-(k)$  as  $\lambda_-(k) = \frac{a_1}{2\nu_2} - \sqrt{k^2 + \delta^2}$  with  $\delta^2 = \frac{a_1^2}{4\nu_2^2} + \frac{\eta_2^2}{\nu_2}$ . Using the dependence on k, the convergence factor becomes 477478

479 
$$\rho(k,\sigma_1,\sigma_2) = \frac{\nu_2\sqrt{k^2+\delta^2} + \frac{a_1}{2} - \sigma_1(k)}{\nu_1\sqrt{\tilde{\eta}_1^2+k^2} + \sigma_1(k)} \frac{\nu_1\sqrt{\tilde{\eta}_1^2+k^2} - \sigma_2(k)}{\nu_2\sqrt{k^2+\delta^2} + \frac{a_1}{2} + \sigma_2(k)}$$

We can define the two optimal operators  $S_j^{\text{opt}}$  associated to the eigenvalues  $\sigma_1^{\text{opt}}(k) := \nu_2 \sqrt{k^2 + \delta^2} + \frac{a_1}{2}$  and  $\sigma_2^{\text{opt}}(k) := \nu_1 \sqrt{k^2 + \tilde{\eta}_1^2}$  which lead to convergence in just two 480481iterations. 482

3.1. Zeroth order single sided optimized transmission conditions. Fol-483 lowing the strategy of the previous section, we choose  $\sigma_1(k), \sigma_2(k)$  so that they coincide 484 with the optimal choice for the frequency k = p, i.e.  $\sigma_1(k) = \nu_2 \sqrt{p^2 + \delta^2} + \frac{a_1}{2}$  and 485 $\sigma_2(k) = \nu_1 \sqrt{p^2 + \tilde{\eta}_1^2}$ . Defining  $\lambda := \frac{\nu_1}{\nu_2}$ , the convergence factor then becomes 486

$$487 \quad (3.2) \quad \rho(k,p) = \frac{\sqrt{k^2 + \tilde{\eta}_1^2} - \sqrt{p^2 + \tilde{\eta}_1^2}}{\frac{1}{\lambda} \left(\sqrt{k^2 + \delta^2} + \frac{a_1}{2\nu_2}\right) + \sqrt{p^2 + \tilde{\eta}_1^2}} \cdot \frac{\sqrt{k^2 + \delta^2} - \sqrt{p^2 + \delta^2}}{\lambda\sqrt{k^2 + \tilde{\eta}_1^2} + \left(\sqrt{p^2 + \delta^2} + \frac{a_1}{2\nu_2}\right)}$$

491

474

489 THEOREM 3.1. The unique optimized Robin parameter  $p^*$  solving the min-max problem 490

$$\min_{p \in \mathbb{R}} \max_{k_{\min} \le k \le k_{\max}} |\rho(k, p)|,$$

is given by the unique root of the non linear equation 492

493 
$$|\rho(p^*, k_{\min})| = |\rho(p^*, k_{\max})|$$

*Proof.* The proof is very similar to the proof of Theorem 2.3, therefore we just 494 sketch the main steps. We start observing that  $\rho(k, p)$  has only one zero located at 495k = p and  $\rho(k, p) > 0$   $\forall k, p$ . Thus we may neglect the absolute value. Analysing the 496derivative with respect to p, we find 497

498 
$$\operatorname{sign}\left(\frac{\partial\rho(k,p)}{\partial p}\right) = -\operatorname{sign}(k-p).$$

This implies that  $\frac{\partial \rho(k,p)}{\partial p} > 0$  if k < p and  $\frac{\partial \rho(k,p)}{\partial p} < 0$  if k > p. We conclude that p must lie in the interval  $[k_{\min}, k_{\max}]$ . Similarly the derivative with respect to k satisfies 499 500

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501  $\frac{\partial_p(k,p)}{\partial k} < 0$  if k < p and  $\frac{\partial_p(k,p)}{\partial k} > 0$  if k > p. Hence, the local maxima with respect 502 to k are located at the boundary points  $k = k_{\min}$  and  $k = k_{\max}$ . Repeating the final 503 argument of Theorem 2.3 we get the result.

Since a closed form formula is again not available, we show now asymptotic results for the optimal parameter  $p^*$  and observe the behaviour of the method when taking finer and finer meshes.

507 THEOREM 3.2. If the physical parameters are fixed,  $k_{\max} = \frac{\pi}{h}$  and h is small enough, 508 then the optimized Robin parameter  $p^*$  satisfies

509 
$$p^* \sim C_a \cdot h^{-\frac{1}{2}}, \ C_a = \frac{\sqrt{\nu_2 (\lambda + 1) \pi \left(2\sqrt{k_{\min}^2 + \tilde{\eta}_1^2}\lambda\nu_2 + 2\sqrt{k_{\min}^2 + \delta^2}\nu_2 - a_1\right)}}{\sqrt{2\nu_2 (\lambda + 1)}}$$

510 Furthermore the asymptotic convergence factor is

511 
$$\max_{k_{\min} \le k \le \pi/h} |\rho(k, p^*)| \sim 1 - h^{\frac{1}{2}} \left( \frac{C_a \left(\lambda + 1\right)^2}{\lambda \pi} \right).$$

512 Proof. We insert the ansatz  $p = C_a \cdot h^{-\alpha}$  into the equation (2.12). Expanding for 513 small h, we get that

514 
$$\rho(p, k_{\min}) \sim 1 - h^{\alpha} \left( \frac{C_a \left( \lambda + 1 \right)^2}{\lambda \pi} \right).$$

515 On the other hand,

516 
$$\rho(p, k_{\max}) \sim 1 + h^{-\alpha+1} \left( \frac{1}{2} \frac{(\lambda+1) \left( -2\sqrt{k_{\min}^2 + \tilde{\eta}_1^2} \lambda \nu_2 - 2\sqrt{k_{\min}^2 \delta^2} \nu_2 + a_1 \right)}{C_a \nu_2 \lambda} \right).$$

517 Comparing the first two terms we get the result.

518 **3.2.** Zeroth order two sided optimized transmission conditions. In this 519 paragraph we generalize the previous transmission conditions, introducing another 520 degree of freedom q. The operators  $S_j$  are such that their eigenvalues are

521 
$$\sigma_1(k) = \nu_2 \sqrt{q^2 + \delta^2} + \frac{a_1}{2}, \qquad \sigma_2(k) = \nu_1 \sqrt{p^2 + \tilde{\eta}_1^2}$$

522 and the convergence factor becomes

523 
$$\rho(k,p) = \frac{\sqrt{k^2 + \tilde{\eta}_1^2} - \sqrt{p^2 + \tilde{\eta}_1^2}}{\frac{1}{\lambda} \left(\sqrt{k^2 + \delta^2} + \frac{a_1}{2\nu_2}\right) + \sqrt{p^2 + \tilde{\eta}_1^2}} \cdot \frac{\sqrt{k^2 + \delta^2} - \sqrt{q^2 + \delta^2}}{\lambda\sqrt{k^2 + \tilde{\eta}_1^2} + \left(\sqrt{q^2 + \delta^2} + \frac{a_1}{2\nu_2}\right)}$$

In order to prove a similar result as in Theorem 2.10, we suppose that  $\tilde{\eta}_1 = 0$ , i.e. only diffusion is present in  $\Omega_1$ , and  $a_1 > 0$ , i.e. the advection flux is pointing into the subdomain  $\Omega_2$ .

527 THEOREM 3.3. There are two pairs of parameters  $(p_1^*, q_1^*)$  and  $(p_2^*, q_2^*)$  such that 528 we obtain equioscillation between all the three local maxima located at the boundary 529 extrema  $k_{\min}, k_{\max}$  and at the interior point  $\hat{k}$ ,

530 
$$|\rho(k_{\min}, p_j^*, q_j^*)| = |\rho(k_{\max}, p_j^*, q_j^*)| = |\rho(k, p_j^*, q_j^*)| \quad j = 1, 2.$$

The optimal pair of parameters is the one which realizes the 531

532 
$$\min_{(p_j^*, q_j^*), j=1,2} |\rho(k_{\min}, p_j^*, q_j^*)|.$$

*Proof.* Similarly to the proof of Theorem 2.10, we observe that the function admits 533 534two zeros, one located at k = p, the other at k = q due to the choice of the transmission operators. Computing the derivatives with respect to p and q we get

$$\operatorname{sign}\left(\frac{\partial|\rho|}{\partial p}\right) = -\operatorname{sign}(\rho) \cdot \operatorname{sign}(k-q) = -\operatorname{sign}(k-p),$$
$$\operatorname{sign}\left(\frac{\partial|\rho|}{\partial q}\right) = -\operatorname{sign}(\rho) \cdot \operatorname{sign}(k-p) = -\operatorname{sign}(k-q).$$

We conclude that, at the optimum, both p and q lie in  $[k_{\min}, k_{\max}]$ , i.e. the function at the optimum has two zeros in the interval. Now we study the behaviour with respect 538 to k. Computing the derivative with respect to k, we find that the potential local 539maxima are given by the roots of 540

541 
$$\frac{\sqrt{\delta^2 + k^2} - \sqrt{\delta^2 + q^2}}{k(\lambda k + \sqrt{q^2 + \delta^2} + \frac{a_1}{2\nu_2})} = \frac{p - k}{\sqrt{k^2 + \delta^2} \left(p\lambda + \sqrt{k^2 + \delta^2} + \frac{a_1}{2\nu_2}\right)}$$

With some algebraic manipulations, we find that a sufficient condition such that  $\frac{p-k}{(p\lambda+\sqrt{k^2+\delta^2}+a_1/(2\nu_2))}$  has a monotonic behaviour with respect to k is that  $a_1 > 0$ . Then under this hypothesis we may repeat the arguments in the proof of Theorem 542 543 5442.10. Letting p, q in  $[k_{\min}, k_{\max}]$ , we have that the local maxima of the function are 545546 located at  $k_{\min}, k_{\max}, k$ . Moreover we have

547 
$$\frac{\partial |\rho|}{\partial p}|_{k=k_{\min}} > 0, \qquad \qquad \frac{\partial |\rho|}{\partial q}|_{k=k_{\min}} > 0,$$
548 (3.3) 
$$\frac{\partial |\rho|}{\partial p}|_{k=k_{\max}} < 0, \qquad \qquad \frac{\partial |\rho|}{\partial q}|_{k=k_{\max}} < 0,$$

548 (3.3) 
$$\frac{\partial |\rho|}{\partial p}|_{k=k_{\max}} < 0,$$

$$\begin{array}{ll} 549\\ 550 \end{array} \qquad \qquad \frac{\partial |\rho|}{\partial p}|_{k=\tilde{k}} < 0, \qquad \qquad \frac{\partial |\rho|}{\partial q}|_{k=\tilde{k}} > 0. \end{array}$$

We can thus repeat the same arguments as in the proof of Theorem 2.10 since all steps are now exclusively based on the sign of the partial derivatives with respect to 552the parameters, see (3.3), and the result follows. 553

THEOREM 3.4. Let  $D := \sqrt{k_{\min}^2 + \delta^2}$ . If the physical parameters  $\tilde{\eta}_2^2, \nu_1, \nu_2, a_1$  are 554fixed,  $k_{\max} = \frac{\pi}{h}$  and h goes to zero, the optimized two-sided Robin parameters are for 555 $\lambda\geq 1,$ 556

557 
$$p_1^* \sim P_1 h^{-1} + E_1 h^{-\frac{1}{2}}, q_1^* \sim Q_1 - F_1 h^{\frac{1}{2}}, \max_{k_{\min} \le k \le \frac{\pi}{h}} |\rho(k, p_1^*, q_1^*)| \sim \lambda - \frac{E_1 \pi (\lambda + 1)}{(P_1 \lambda + \pi)^2} h^{\frac{1}{2}},$$

558 with

559 
$$P_{1} := \frac{\pi(\lambda - 1)}{2\lambda}, \quad Q_{1} := \sqrt{\frac{D + k_{\min} + \frac{a_{1}}{2\nu_{2}\lambda}}{1 - \frac{1}{\lambda}}} - \delta^{2},$$
  
560 
$$E_{1} := \frac{(2(P_{1}\sqrt{\delta^{2} + Q_{1}^{2}} + C_{h}^{2})(\lambda + 1)\nu_{2} + P_{1}a_{1})(\lambda P_{1} + \pi)^{2}}{2\lambda^{2}P_{1}\nu_{2}C_{h}\pi(\lambda + 1)},$$

561 
$$F_1 := \frac{(2(P_1\sqrt{\delta^2 + Q_1^2} + C_h^2)(\lambda + 1)\nu_2 + P_1a_1)(2\nu_2(\lambda k_{\min} + \sqrt{\delta^2 + Q_1^2}) + a_1)^2\sqrt{\delta^2 + Q_1^2}}{4\lambda^2 P_1\nu_2^2 C_h Q_1(2\nu_2(\lambda k_{\min} + D) + a_1)}$$

562 
$$C_h := \frac{\sqrt{P_1(2\sqrt{\delta^2 + Q_1^2}\nu_2(\lambda+1) + a_1)}}{\sqrt{2\nu_2(\lambda+1)}}$$

564 and for  $\lambda < 1$ ,

565 
$$p_2^* \sim P_2 - E_2 h^{\frac{1}{2}}, q_2^* \sim Q_2 h^{-1} + F_2 h^{-\frac{1}{2}}, \max_{k_{\min} \le k \le \frac{\pi}{h}} |\rho(k, p_2^*, q_2^*)| \sim \lambda - \frac{F_2 \lambda \pi (1+\lambda)}{(\lambda \pi + Q_2)^2} h^{\frac{1}{2}}.$$

566 with

567 
$$P_2 := \frac{D}{2}$$

$$P_{2} := \frac{D + k_{\min} + \frac{a_{1}}{2\nu_{2}}}{1 - \lambda}, \quad Q_{2} := \frac{\pi(\lambda - 1)}{2},$$

$$E_{2} := \frac{((\lambda + 1)(D_{h}^{2} + P_{2}Q_{2})\nu_{2} + \frac{a_{1}Q_{2}}{2})(2\nu_{2}(\lambda P_{2} + D) + a_{1})^{2}}{2\nu_{2}^{2}D_{h}Q_{2}(2k_{\min}\lambda\nu_{2} + 2\nu_{2}D + a_{1})}$$

$$= \sqrt{\lambda + 1} \sqrt{(D + k_{\perp})(\lambda + 1) + \frac{a_{1}}{2}} \sqrt{\pi(3\lambda - 1)^{2}}$$

$$F_2 := \frac{\sqrt{\lambda + 1}\sqrt{(D + k_{\min})(\lambda + 1) + \frac{a_1}{2\nu_2}\sqrt{\pi}(3\lambda - \sqrt{2})}}{\sqrt{2}(1 - \lambda^2)}$$
$$D_h := \frac{\sqrt{Q_2(2P_2\nu_2(\lambda + 1) + a_1)}}{\sqrt{2\nu_2(\lambda + 1)}}.$$

$$570 \\ 571$$

572 *Proof.* The proof follows the same steps as in the proof of Theorem 2.11.

**3.3.** Advection tangential to the interface. In the previous subsection we 573 restricted our study to the case of advection normal to the interface. Here we consider 574the other relevant physical case, namely advection tangential to the interface, so that  $a_1 = 0$  and  $a_2 \neq 0$  in (3.1). For homogeneous problems, this case has been studied 576through Fourier transform in unbouded domains, see for instance [7]. However, it 577has recently been observed in [18], that for homogeneous problems with tangential 578advection this procedure does not yield efficient optimized parameters. The reason 579behind this failure lies in the separation of variables technique which applied to the 580error equation, 581

$$(\eta_1^2 - \nu_1 \Delta) e_1^n = 0, \text{ in } \Omega_1, (\nu_1 \partial_x + S_1)(e_1^n)(0, \cdot) = (\nu_2 \partial_x + S_1)(e_2^{n-1})(0, \cdot), (\eta_2^2 + a_2 \partial_y - \nu_2 \Delta) e_2^n = 0, \text{ in } \Omega_2, (\nu_2 \partial_x - S_2)(e_2^n)(0, \cdot) = (\nu_1 \partial_x - S_2)(e_1^{n-1})(0, \cdot),$$

583 leads to

584 (3.5) 
$$e_1^n = \sum_{k \in \mathcal{V}} \hat{e}_1^n(0,k) e^{\lambda_1(k)x} \sin(ky)$$
 and  $e_2^n = \sum_{k \in \mathcal{V}} \hat{e}_2^n(0,k) e^{-\lambda_2(k)x} e^{\frac{a_2y}{2\nu_2}} \sin(ky),$ 

where  $\lambda_1(k) = \sqrt{k^2 + \tilde{\eta_1}}$ ,  $\lambda_2(k) = \frac{\sqrt{4\nu_2^2 k^2 + 4\nu_2^2 \tilde{\eta_2}^2 + a_2^2}}{2\nu_2}$  with  $\tilde{\eta}_j^2 := \frac{\eta_j^2}{\nu_j}$ . Since the functions  $\psi_k(y) := \sin(ky)$  and  $\phi_k(y) := e^{\frac{a_2y}{2\nu_2}} \sin(ky)$  are not orthogonal, it is not possible

to obtain a recurrence relation which expresses  $\hat{e}_j^n(0,k)$  only as a function of  $\hat{e}_j^{n-2}(0,k)$ 587

for each k and j = 1, 2. Nevertheless we here propose a more general approach. First 588

let us define two scalar products, the classical  $L^2$  scalar product  $\langle f, g \rangle = \frac{2}{L} \int_{\Gamma} fg dy$  and 589

the weighted scalar product  $\langle f, g \rangle_{\mathbf{w}} = \frac{2}{L} \int_{\Gamma} fg e^{-\frac{a_2 y}{\nu_2}} dy$ . It follows that  $\langle \psi_k, \psi_j \rangle = \delta_{k,j}$ and  $\langle \phi_k, \phi_j \rangle_{\mathbf{w}} = \delta_{k,j}$ . Setting  $S_1 := \nu_2 \lambda_2(p)$  and  $S_2 := \nu_1 \lambda_1(q)$  for  $p, q \in \mathbb{R}$  and 590

591

inserting the expansions (3.5) into the boundary conditions of (3.4) we obtain 592 (3.6)

593

$$\sum_{i=1}^{+\infty} \hat{e}_1^n(0,i)(\nu_1\lambda_1(i)+\nu_2\lambda_2(p))\psi_i(y) = \sum_{l=1}^{+\infty} \hat{e}_2^{n-1}(0,l)(-\nu_2\lambda_2(l)+\nu_2\lambda_2(p))\phi_l(y),$$
  
$$\sum_{l=1}^{+\infty} \hat{e}_2^n(0,l)(-\nu_2\lambda_2(l)-\nu_1\lambda_1(q))\phi_l(y) = \sum_{i=1}^{+\infty} \hat{e}_1^{n-1}(0,i)(\nu_1\lambda_1(i)-\nu_1\lambda_1(q))\psi_i(y).$$

We truncate the expansions for i, l > N, since higher frequencies are not represented by the numerical grid, and we project the first equation onto  $\psi_k$  with respect the scalar product  $\langle \cdot, \cdot \rangle$  and the second one onto  $\phi_i$  with respect to the weighted scalar 596 product  $\langle \cdot, \cdot \rangle_{w}$ ,

(3.7)

598

$$\hat{e}_{1}^{n}(0,k)(\nu_{1}\lambda_{1}(k)+\nu_{2}\lambda_{2}(p)) = \sum_{l=1}^{N} \hat{e}_{2}^{n-1}(0,l)(-\nu_{2}\lambda_{2}(l)+\nu_{2}\lambda_{2}(p))\langle\psi_{k},\phi_{l}\rangle,$$
$$\hat{e}_{2}^{n}(0,j)(-\nu_{2}\lambda_{2}(j)-\nu_{1}\lambda_{1}(q)) = \sum_{i=1}^{N} \hat{e}_{1}^{n-1}(0,i)(\nu_{1}\lambda_{1}(i)-\nu_{1}\lambda_{1}(q))\langle\phi_{j},\psi_{i}\rangle_{w}.$$

Defining now the vectors  $\mathbf{e}_j^n \in \mathbb{R}^N$  such that  $(\mathbf{e}_j^n)_i := \hat{e}_j^n(0,i)$  for j = 1, 2, the matrices 599 $V_{k,l} := \langle \psi_k, \phi_l \rangle, W_{j,i} := \langle \phi_j, \psi_i \rangle_w$  and the diagonal matrices  $(D_1)_{l,l} := (-\nu_2 \lambda_2(l) + \nu_2 \lambda_2(l))$ 600  $\nu_2\lambda_2(p)), (\tilde{D}_1)_{k,k} := (\nu_1\lambda_1(k) + \nu_2\lambda_2(p)), (D_2)_{i,i} := (\nu_1\lambda_1(i) - \nu_1\lambda_1(q)), (\tilde{D}_2)_{j,j} := (\nu_1\lambda_1(k) + \nu_2\lambda_2(p)), (D_2)_{i,j} := (\nu_1\lambda_1(k)$ 601602  $(-\nu_2\lambda_2(j)-\nu_1\lambda_1(q))$ , we obtain,

603 (3.8) 
$$\mathbf{e}_{1}^{n} = \tilde{D}_{1}^{-1} V D_{1} \mathbf{e}_{2}^{n-1}, \\ \mathbf{e}_{2}^{n} = \tilde{D}_{2}^{-1} W D_{2} \mathbf{e}_{1}^{n-1},$$

which implies 604

605 (3.9) 
$$\mathbf{e}_1^n = \tilde{D}_1^{-1} V D_1 \tilde{D}_2^{-1} W D_2 \mathbf{e}_1^{n-2} \text{ and } \mathbf{e}_2^n = \tilde{D}_2^{-1} W D_2 \tilde{D}_1^{-1} V D_1 \mathbf{e}_2^{n-2}.$$

Since for two given matrices A, B the spectral radius satisfies  $\rho(AB) = \rho(BA)$ , we 606 conclude that  $\rho(\tilde{D}_1^{-1}VD_1\tilde{D}_2^{-1}WD_2) = \rho(\tilde{D}_2^{-1}WD_2\tilde{D}_1^{-1}VD_1)$  and therefore, in order 607 to accelerate the method, we are interested in the minimization problem 608

609 (3.10) 
$$\min_{p,q \in \mathbb{R}} \rho((\tilde{D}_1^{-1}VD_1\tilde{D}_2^{-1}WD_2)(p,q)).$$

Problem (3.10) does not have vet a closed formula solution. However in the next 610 section we show its efficiency by solving numerically the minimization problem. 611

Remark 3.5. Equation (3.10) is a straight generalization of the min-max prob-612 lem (2.8). Indeed, assuming that the functions  $\psi_k$  and  $\phi_i$  are orthogonal, the ma-613 trices V and W are the identity matrix. Therefore equation (3.9) simplifies to  $\mathbf{e}_1^n = \bar{D}\mathbf{e}_1^{n-2}$  and  $\mathbf{e}_2^n = \bar{D}\mathbf{e}_2^{n-2}$ , where the diagonal matrix  $\bar{D}$  satisfies  $(\bar{D})_{k,k} = \frac{\nu_2\lambda_2(k)-\nu_2\lambda_2(p)}{\nu_1\lambda_1(k)+\nu_2\lambda_2(p)}\frac{\nu_1\lambda_1(k)-\nu_1\lambda_1(q)}{\nu_2\lambda_2(k)+\nu_1\lambda_1(q)}$ . Since the eigenvalues of a diagonal matrix are its diagonal entries we get that if W = V = I, 614 615 616 617

618 
$$\min_{p,q \in \mathbb{R}} \rho((\tilde{D}_1^{-1}VD_1\tilde{D}_2^{-1}WD_2)(p,q)) = \min_{p,q} \max_k \left| \frac{\nu_2 \lambda_2(k) - \nu_2 \lambda_2(p)}{\nu_1 \lambda_1(k) + \nu_2 \lambda_2(p)} \frac{\nu_1 \lambda_1(k) - \nu_1 \lambda_1(q)}{\nu_2 \lambda_2(k) + \nu_1 \lambda_1(q)} \right|.$$

h	$\rho$ single sided	$\rho$ double sided	h	$\rho$ single sided	$\rho$ double sided
1/50	0.7035	0.4052	1/50	0.1721	0.0337
1/100	0.7801	0.4748	1/100	0.2625	0.0456
1/500	0.8950	0.6160	1/500	0.4868	0.0685
1/1000	0.9245	0.6672	1/1000	0.5823	0.0760
1/5000	0.9655	0.7650	1/5000	0.7662	0.0872

Table 2: Asymptotic behaviour as  $h \to 0$  for the reaction diffusion-diffusion coupling. Physical parameters: left table  $\tilde{\eta}^2 = \lambda = 1$ , right table  $\tilde{\eta}^2 = \lambda = 10$ .

619 Remark 3.6. The case of an arbitrary advection, i.e.  $a_1 \neq 0$  and  $a_2 \neq 0$  has 620 been recently treated in [18] for homogeneous problems. Considering a heterogeneous 621 problem with advection fields  $\mathbf{a}_j = (a_{1j}, a_{2j})^{\top}$  in domain  $\Omega_j$ , j = 1, 2, a separation 622 of variables approach would lead to non orthogonal functions  $\psi_k(y) = e^{\frac{a_{21}y}{2\nu_1}} \sin(ky)$ 623 and  $\phi_k(y) = e^{\frac{a_{22}y}{2\nu_2}} \sin(ky)$  unless  $\frac{a_{21}}{2\nu_1} = \frac{a_{22}}{2\nu_2}$ , and thus it is not possible to obtain a 624 recurrence relation as shown in (3.5). However the approach developed in this section 625 can be readily applied. The subdomain solutions are

626 
$$e_1^n(x,y) = \sum_{k \in \mathcal{V}} \hat{e}_{1,k}^n e^{\frac{a_{21}y}{2\nu_1}} \sin(ky) e^{\lambda_1(k)x}, \quad e_2^n(x,y) = \sum_{k \in \mathcal{V}} \hat{e}_{2,k}^n e^{\frac{a_{22}y}{2\nu_2}} \sin(ky) e^{-\lambda_2(k)x}.$$

627 with  $\lambda_1(k) = \frac{a_{11} + \sqrt{4\nu_1^2 k^2 + 4\nu_1^2 \tilde{\eta}_1^2 + a_{11}^2 + a_{21}^2}}{2\nu_1}$  and  $\lambda_2(k) = \frac{-a_{12} + \sqrt{4\nu_2^2 k^2 + 4\nu_2^2 \tilde{\eta}_2^2 + a_{12}^2 + a_{22}^2}}{2\nu_2}$ . 628 Defining  $S_1 = \nu_2 \lambda_2(p) + a_{12}, S_2 = \nu_1 \lambda_1(p) - a_{11}$ , the two scalar products  $\langle f, g \rangle_{w_1} = \frac{2}{L} \int_{\Gamma} fg e^{-\frac{a_{21}y}{\nu_1}} dy$  and  $\langle f, g \rangle_{w_2} = \frac{2}{L} \int_{\Gamma} fg e^{-\frac{a_{22}y}{\nu_2}} dy$  and repeating the calculations (3.6)-630 (3.8), one finds the recurrence relation (3.9), with  $V_{k,l} := \langle \psi_k, \phi_l \rangle_{w_1}, W_{j,i} := \langle \phi_j, \psi_i \rangle_{w_2}$ 631 and the diagonal matrices  $(D_1)_{l,l} := (-\nu_2 \lambda_2(l) + \nu_2 \lambda_2(p)), (\tilde{D}_1)_{k,k} := (\nu_1 \lambda_1(k) + \nu_2 \lambda_2(p) - a_{11} + a_{12}), (D_2)_{i,i} := (\nu_1 \lambda_1(i) - \nu_1 \lambda_1(q)), (\tilde{D}_2)_{j,j} := (-\nu_2 \lambda_2(j) - \nu_1 \lambda_1(q) - a_{12} + a_{11}).$ 

634 **4.** Numerical results. Our numerical experiments to test the different coupling 635 strategies separately are performed using the subdomains  $\Omega_1 = (-1, 0) \times (0, 1)$ ,  $\Omega_2 =$ 636  $(0, 1) \times (0, 1)$ . We use a classical five point finite difference scheme for the interior 637 points and treat the normal derivatives with second order discretization using a ghost 638 point formulation.

4.1. Reaction Diffusion-Diffusion coupling. We first consider the reaction 639 diffusion-diffusion coupling analyzed in Section 2. Tables 2 and 3 show the values 640 of the convergence factor in two different asymptotic regimes, when  $h \to 0$ , and 641 for strong heterogeneity. As the asymptotic Theorem 2.11 and Remark 2.5 state, a 642 643 strong heterogeneity improves the performance of the algorithm. In the single sided optimized case, the value of the convergence factor  $|\rho(k)|$  tends to 1, while in the 644 double sided case,  $|\rho(k)|$  is bounded either by  $\lambda$  or by  $1/\lambda$ . Fig. 4 shows the number 645 of iterations required to reach convergence with a tolerance of  $10^{-6}$  as function of 646 the optimized parameters in both the single and double sided cases. We see that the 647 648 analysis predicts the optimized parameter very well.

649 **4.2.** Advection Reaction Diffusion-Diffusion coupling. Next we consider 650 the advection reaction diffusion-diffusion coupling with advection normal to the inter-651 face. Table 4 summarizes the behaviour of  $\rho(k)$  as  $h \to 0$  and for strong heterogeneity.

$\lambda$	$\rho$ single sided	$\rho$ double sided
0.001	0.0125	$7.8 \cdot 10^{-4}$
0.01	0.1075	0.0078
0.1	0.4453	0.0757
1	0.5851	0.4748
10	0.2625	0.076
100	0.0389	0.0078
1000	0.0040	$7.8 \cdot 10^{-4}$

Table 3: Asymptotic behaviour as  $\lambda \to 0$  and  $\lambda \to \infty$ , with h = 0.05 for the reaction diffusion-diffusion coupling. Physical parameter:  $\tilde{\eta}^2 = 1$ .



Fig. 4: Number of iterations required to reach convergence with a tolerance of  $10^{-6}$  as function of the optimized parameters for the reaction diffusion-diffusion coupling. The left panel shows the single sided case while the right panel shows the double sided case. Physical parameters :  $\nu_1 = 2$ ,  $\nu_2 = 1$ ,  $\eta^2 = 10$ , mesh size h = 0.02.

Similarly Fig 5 shows the number of iterations required to reach convergence with the tolerance of  $10^{-6}$ . Figure 6 shows the number of iterations to reach convergence for the tangential advection case. The minimization problem (3.10) is solved numerically to find the optimal parameters p and q using the Nelder-Mead algorithm. We have solved the minimization problem with different initial couples (p, q) and we have noticed that the optimal solution satisfies an ordering relation between p and q depending on  $\lambda$  as in Theorem 2.11 and 3.4.

4.3. Application to the contaminant transport problem. The computational domain  $\Omega$  described in Fig 1 is set equal to  $\Omega = (0,8) \times (-4,0)$ , with  $\Omega_j = (0,8) \times (1-j,-j), j = 1...4$ . On the top boundary  $\Gamma_1$ , we impose a condition on the incoming contaminant flow, i.e.  $\frac{\partial u}{\partial y} - a_2 u = 1$  while on the bottom edge  $\Gamma_3$  we impose a zero Neumann boundary condition  $\frac{\partial u}{\partial y} = 0$ . On the vertical edges  $\Gamma_2$ and  $\Gamma_4$  we set absorbing boundary conditions so that

$$\frac{\partial u}{\partial \mathbf{n}} + pu = 0 \quad \text{on} \quad \{0\} \times [-3;0] \text{ and } \{8\} \times [-3;0],$$
  
$$\frac{\partial u}{\partial \mathbf{n}} - a_1 u + pu = 0 \quad \text{on} \quad \{0\} \times [-4;-3] \text{ and } \{8\} \times [-4;-3],$$

			$\lambda$	$\rho$ single sided	$\rho$ double sided
h	$\rho$ single sided	$\rho$ double sided	0.001	0.0031	$4.89 \cdot 10^{-4}$
1/50	0.4766	0.1835	0.01	0.0297	0.0049
1/100	0.5910	0.2306	0.1	0.2101	0.0458
1/500	0.7889	0.3274	1	0.4865	0.2552
1/1000	0.8452	0.3618	10	0.2786	0.0517
1/5000	0.9273	0.4228	100	0.0459	0.0056
			1000	0.0049	$5.6 \cdot 10^{-4}$

Table 4: For the advection reaction diffusion-diffusion coupling, the left table shows the asymptotic behaviour when  $h \to 0$  while the right table shows the values of the convergence factor for strong heterogeneity when h = 1/50. Physical parameters:  $\eta_1^2 = 1, \eta_2^2 = 2, \nu_1 = 2, \nu_2 = 1, a_2 = 0, a_1 = 5$ , mesh size h = 0.02.



Fig. 5: Number of iterations required to reach convergence with a tolerance of  $10^{-6}$  as function of the optimized parameters for the advection reaction diffusion-diffusion coupling with normal advection. Physical parameters:  $\nu_1 = 2$ ,  $\nu_2 = 1$ ,  $\eta_1^2 = 1$ ,  $\eta_2^2 = 2$ ,  $a_1 = 5$ , mesh size h = 0.02.

- 666 where **n** is the outgoing normal vector. The parameter p is chosen equal to  $p = \sqrt{\pi \frac{\pi}{h}}$ , 667 being  $k_{\min} = \pi$  and  $k_{\max} = \frac{\pi}{h}$ . This choice derives from the observation that imposing
- 668  $\frac{\partial u}{\partial n} + DtNu = 0$ , where DtN is the Dirichlet to Neumann operator, is an exact
- 669 transparent boundary condition, see [29, 28]. Thus we replace the expensive exact
- 670 transparent boundary condition with an approximation of the DtN operator. We
- 671 know from [9] that  $p = \sqrt{\pi \frac{\pi}{h}}$  is indeed a zero order approximation of the DtN



Fig. 6: In the top row, we show the number of iterations required to reach convergence with a tolerance of  $10^{-6}$  as function of the optimized parameters for the advection reaction diffusion-diffusion coupling with tangential advection. In the bottom row, we show the dependence on p and the level curves of the objective function in the minmax problem (3.10). Physical parameters:  $\nu_1 = 1$ ,  $\nu_2 = 2$ ,  $\eta_1^2 = 1$ ,  $\eta_2^2 = 2$ ,  $a_2 = 15$ , mesh size h = 0.01.

 $_{(4.1)}$  operator. To solve the system of PDEs, we consider the optimized Schwarz method: (4.1)

$$\begin{array}{c} -\nu_{1}\Delta u_{1}^{n} - a_{2}\partial_{y}u_{1}^{n} = 0 & \text{in }\Omega_{1}, \quad \mathcal{B}_{1}(u_{1}^{n}) = 0 \text{ on }\partial\Omega_{1} \setminus \Sigma_{1}, \\ \partial_{n_{1,2}}u_{1}^{n} + p_{12}u_{1}^{n} = \partial_{n_{1,2}}u_{2}^{n-1} + p_{12}u_{2}^{n-1} & \text{on }\Sigma_{1}, \\ \eta_{2}^{2}u_{2}^{n} - \nu_{2}\Delta u_{2}^{n} = 0 & \text{in }\Omega_{2}, \quad \mathcal{B}_{2}(u_{2}^{n}) = 0 \text{ on }\partial\Omega_{2} \setminus \{\Sigma_{1}, \Sigma_{2}\}, \\ \partial_{n_{1,1}}u_{2}^{n} + p_{21}u_{2}^{n} = \partial_{n_{2,1}}u_{3}^{n-1} + p_{21}u_{1}^{n-1} & \text{on }\Sigma_{1}, \\ \partial_{n_{2,3}}u_{2}^{n} + p_{23}u_{2}^{n} = \partial_{n_{2,3}}u_{3}^{n-1} + p_{23}u_{3}^{n-1} & \text{on }\Sigma_{2}, \\ -\nu_{3}\Delta u_{3}^{n} = 0 & \text{in }\Omega_{3}, \quad \mathcal{B}_{3}(u_{3}^{n}) = 0 \text{ on }\partial\Omega_{3} \setminus \{\Sigma_{2}, \Sigma_{3}\}, \\ \partial_{n_{2,2}}u_{3}^{n} + p_{32}u_{3}^{n} = \partial_{n_{2,2}}u_{2}^{n-1} + p_{32}u_{2}^{n-1} & \text{on }\Sigma_{2}, \\ \partial_{n_{3,4}}u_{3}^{n} + p_{34}u_{3}^{n} = \partial_{n_{3,4}}u_{4}^{n-1} + p_{34}u_{4}^{n-1} & \text{on }\Sigma_{3}, \\ -\nu_{4}\Delta u_{4}^{n} + a_{1}\partial_{x}u_{4}^{n} = 0 & \text{in }\Omega_{4}, \quad \mathcal{B}_{4}(u_{4}^{n}) = 0 \text{ on }\partial\Omega_{4} \setminus \Sigma_{3}, \\ \partial_{n_{3,3}}u_{4}^{n} + p_{43}u_{4}^{n} = \partial_{n_{3,3}}u_{3}^{n-1} + p_{43}u_{3}^{n-1} & \text{on }\Sigma_{3}, \end{array} \right.$$

674 where  $\Sigma_i$  are the shared interfaces  $\Sigma_i = \partial \Omega_i \cap \partial \Omega_{i+1}$ , i = 1, 2, 3, the vectors  $\mathbf{n}_{i,j}$  are 675 the normal vectors on the interface  $\Sigma_i$  pointing towards the interior of the domain  $\Omega_j$ 676 and the operators  $\mathcal{B}_i(u_i)$  represent the boundary conditions to impose on the bound-677 ary excluding the shared interfaces. Regarding the Robin parameters  $p_{i,j}$ , we choose



Stationary distribution of the contaminant. Physical parameters:  $\nu_1 = 0.5, \nu_2 = 3, \nu_3 = 3, \nu_4 = 1, \eta_2^2 = 0.01, a_2 = 2, a_1 = 2.$ 

678 them according to the two subdomain analysis carried out in this manuscript. Due to the exponential decay of the error away from the interface, see eq. (2.3), if the 679 subdomains are not too narrow in the y direction, the information transmitted from 680 each subdomain to the neighbouring one does not change significantly and therefore 681 the  $p_{i,j}$  from a two subdomain analysis are still a good choice. We remark that this ar-682 gument does not hold for the Helmholtz equation, for which there are resonant modes 683 for frequencies  $k \leq \omega$ , where  $\omega$  is the wave number, which travel along the domains 684 and they do not decay away from the interface. Figure 7 shows the stationary distri-685 bution of the contaminant. We observe that due to the advection in the y direction 686 687 in  $\Omega_1$ , the contaminant accumulates on the interface with  $\Omega_2$ , representing the porous medium, and here we have the highest concentration. Then the contaminant diffuses 688 into the layers below and already in the porous media region it feels the presence of 689 the tangential advection in  $\Omega_4$ . Next we also consider the transient version of equa-690 tions (4.1). We discretize the time derivative with an implicit Euler scheme, so that 691 each equation has a further reaction term equal to  $\eta_{j,tran}^2 = \eta_{j,stat}^2 + \frac{1}{\Delta t}$ . Figure 8 shows the time dependent evolution of the concentration u over 400 integration steps. 692 693 The initial condition is set equal to zero on the whole domain  $\Omega$ . 694

Table 5 shows the number of iterations to reach a tolerance of  $10^{-6}$  for the algorithm (4.1) both used as iterative method and as a preconditioner for GMRES for the substructured system, see [13] for an introduction to the substructured version of (4.1). We consider both single and double sided optimizations for the parameters  $p_{i,j}$ at each interface. For the time evolution problem, the stopping criterion is

700 (4.2) 
$$\max\left\{\frac{\|u_{1,\Sigma_{1}}^{n,k}-u_{2,\Sigma_{1}}^{n,k}\|}{\|u_{1,\Sigma_{1}}^{n,k}\|}, \frac{\|u_{2,\Sigma_{2}}^{n,k}-u_{3,\Sigma_{2}}^{n,k}\|}{\|u_{2,\Sigma_{2}}^{n,k}\|}, \frac{\|u_{3,\Sigma_{1}}^{n,k}-u_{4,\Sigma_{3}}^{n,k}\|}{\|u_{3,\Sigma_{3}}^{n,k}\|}\right\} \le 10^{-6}.$$

From Figures 7 and 8, we note that this physical configuration would represent a safe situation since a very small concentration of contaminant manages to get through the vertical diffusive layers and to reach the right-bottom of the domain, where it could pollute the water well.

**5.** Conclusions. In this manuscript we considered the heterogeneous couplings arising from second order elliptic PDEs and solved analytically the corresponding



Fig. 8: Evolution of the contaminant concentration u.

	Iterative	GMRES		Iterative	GMRES
Single sided	270	33	Single sided	11.5	5.7
Double sided	55	25	Double sided	9.6	4.3

Tal	ble	5
T COL	010	<u> </u>

Number of iterations to reach a tolerance of  $10^{-6}$  for the optimized Schwarz method (4.1) used as an iterative method and as a preconditioner. The left side refers to the stationary case while the right side to the transient one where we consider the

number of iterations needed to satisfy the stopping criterion (4.2) averaged over 400 time steps.

707 min-max problems, except in the case of tangential advection to the interface where 708 we provided a numerical optimization procedure. Our results show that optimized Schwarz methods are not only natural for heterogeneous problems, they are also ex-709 710 tremely efficient. Indeed, the asymptotic analysis shows that the stronger the heterogeneity is, the fastest becomes the convergence. In particular, a double sided method 711 712 should be preferred since not only is it clearly faster than a single sided one, but it 713 also leads to an h independent convergence as long as there is a jump in the diffusion coefficients. Our analysis is based on a two dimensional setting but the results can be 714extended to three dimensional problems. Considering  $\Omega_1 = (-\infty, 0) \times (0, L) \times (0, \hat{L})$ 715716 and  $\Omega_2 = (0, +\infty) \times (0, L) \times (0, L)$ , we can obtain analogous sine expansions for the

errors  $e_i^n$ , j = 1, 2 as in Section 2. Then, for symmetric problems and in the case of 717 normal advection to the plane  $\Gamma := \{0\} \times (0, L) \times (0, \hat{L})$ , we can reuse the same theo-718 retical results by changing the range of frequencies in the min-max problems, setting 719  $k_{\min} = \frac{\pi}{L} + \frac{\pi}{\tilde{L}}$  and  $k_{\max} = \frac{2\pi}{h}$ . Considering tangential advection, all the possible tan-720 gential directions now lie on the plane  $\Gamma$ , which in our example is the y-z plane. Then 721 one could use the numerical procedure developed in Section 3.3 introducing the ma-722 trices V and W and proper scalar products defined as integrals on the 2 dimensional 723 724 interface.

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