NEW TIME DOMAIN DECOMPOSITION METHODS FOR PARABOLIC OPTIMAL CONTROL PROBLEMS I: DIRICHLET-NEUMANN AND NEUMANN-DIRICHLET ALGORITHMS*

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Abstract. We present new Dirichlet-Neumann and Neumann-Dirichlet algorithms with a time domain decomposition applied to unconstrained parabolic optimal control problems. After a spatial semi-discretization, we use the Lagrange multiplier approach to derive a coupled forward-backward optimality system, which can then be solved using a time domain decomposition. Due to the forward-backward structure of the optimality system, three variants can be found for the Dirichlet-Neumann and Neumann-Dirichlet algorithms. We analyze their convergence behavior and determine the optimal relaxation parameter for each algorithm. Our analysis reveals that the most natural algorithms are actually only good smoothers, and there are better choices which lead to efficient solvers. We illustrate our analysis with numerical experiments.

Key words. Time domain decomposition, Dirichlet-Neumann algorithm, Neumann-Dirichlet algorithm, Parallel in Time, Parabolic optimal control problems, Convergence analysis.

MSC codes. 65M12,65M55,65Y05,

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1. Introduction. PDE-constrained optimal control problems arise in various areas, often containing multiphysics or multiscale phenomena, and also high frequency components on different time scales. This requires very fine spatial and temporal discretizations, resulting in very large problems, for which efficient parallel solvers are needed; we refer to [14, 26] for a brief review. We present and analyze a new class of time domain decomposition methods based on Dirichlet-Neumann and Neumann-Dirichlet techniques. We consider as our model a parabolic optimal control problem: for a given target function $\hat{y} \in L^2(Q)$, $\gamma \geq 0$ and $\nu > 0$, we want to minimize the cost functional

$$J(y,u) := \frac{1}{2} \|y - \hat{y}\|_{L^2(Q)}^2 + \frac{\gamma}{2} \|y(T) - \hat{y}(T)\|_{L^2(\Omega)}^2 + \frac{\nu}{2} \|u\|_{U_{ad}}^2,$$

subject to the linear parabolic state equation

$$\partial_t y - \Delta y = u \qquad \text{in } Q := \Omega \times (0, T),$$

$$y = 0 \qquad \text{on } \Sigma := \partial \Omega \times (0, T),$$

$$y(0) = y_0 \qquad \text{on } \Sigma_0 := \Omega \times \{0\},$$

where $\Omega \subset \mathbb{R}^d$, d=1,2,3 is a bounded domain with boundary $\partial\Omega$, and T is the fixed final time. The control u on the right-hand side of the PDE is in an admissible set $U_{\rm ad}$, and we want to control the solution of the parabolic PDE (1.2) towards a target state \hat{y} . For simplicity, we consider here homogeneous boundary conditions.

The parabolic optimal control problem (1.1)-(1.2) has a unique solution for the classical choice $u \in L^2(Q)$, which can be characterized by a forward-backward optimality system, see e.g. [4, 18, 26]. More recently, also energy regularization has been considered, see [23] for elliptic and [16] for parabolic cases. This is motivated by

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the fact that the state $y \in L^2(0,T;H_0^1(\Omega))$ is well-defined as the solution of the heat equation (1.2) for the control $z \in L^2(0,T;H^{-1}(\Omega))$, and thus offers an interesting alternative.

We are interested in applying Time Domain Decomposition methods (DDMs) to the forward-backward optimality system. DDMs were developed for elliptic PDEs and are very efficient in parallel computing environments, see e.g. [7, 25]. DDMs were extended to time-dependent problems using waveform relaxation techniques from [17], with a spatial decomposition and solving the problem on small space-time cylinders [12]. The extension of DDMs to elliptic optimal control problems is quite natural, see [1, 2, 5, 9], but less is known about DDMs applied to parabolic optimal control problems.

The role of the time variable in forward-backward optimality systems is key, and it is natural to seek efficient solvers through time domain decomposition. For classical evolution problems, the idea of time domain decomposition goes back to [24]. Parallel Runge Kutta methods were introduced in [22] with good small scale time parallelism. In [20, 27], the authors propose to combine multigrid methods with waveform relaxation. Parareal [19] uses a different approach, namely multiple shooting with an approximate Jacobian on a coarse grid, and Parareal techniques led to a new ParaOpt algorithm [10] for optimal control, see also [13]. In [8, 15], Schwarz methods are used to decompose the time domain for optimal control. Waveform relaxation techniques can also be applied to address such optimal control problems, for instance, using Dirichlet-Neumann waveform relaxation methods [21] and Optimized Schwarz waveform relaxation methods [6]. Note that the decomposition in [6, 21] is in space of the PDE constraint, in contrast to the approach presented in [8, 15], and also in contrast to our approach in time here.

We develop and analyze here new time domain decomposition algorithms to solve the PDE-constrained problem (1.1)-(1.2) using Dirichlet-Neumann and Neumann-Dirichlet techniques that go back to [3] for space parallelism. We introduce in Section 2 the optimality system and its semi-discretization. In Section 3 we present our new time parallel Dirichlet-Neumann and Neumann-Dirichlet algorithms and study their convergence. Numerical experiments are shown in Section 4, and we draw conclusions in Section 5.

2. Optimality system and its semi-discretization. The PDE-constrained optimization problem (1.1)-(1.2) can be solved using Lagrange multipliers [26, Chapter 3], see also [11] for a historical context. To obtain the associated optimality system, we introduce the Lagrangian function \mathcal{L} associated with Problem (1.1)-(1.2),

$$\mathcal{L}(y, u, \lambda) = J(y, u) + \langle \partial_t y - \Delta y - u, \lambda \rangle$$

$$= \int_0^T \left(\langle \partial_t y, \lambda \rangle_{V', V} + \int_{\Omega} \left(\frac{1}{2} |y - \hat{y}|^2 + \frac{\nu}{2} |u|^2 + \nabla y \cdot \nabla \lambda - u\lambda \right) d\mathbf{x} \right) dt$$

$$+ \frac{\gamma}{2} \int_{\Omega} |y(T) - \hat{y}(T)|^2 d\mathbf{x},$$

with $y \in W(0,T) := L^2(0,T;V) \cap H^1(0,T;V')$, $u \in L^2(Q)$, $V := H^1_0(\Omega)$ and $V' := H^{-1}(\Omega)$ the dual space of V. Here $\lambda \in L^2(0,T;V)$ denotes the adjoint state (also called the Lagrange multiplier). Taking the derivative of \mathcal{L} with respect to λ and equating this to zero, we find for all test functions $\chi \in L^2(0,T;V)$,

$$0 = \langle \partial_{\lambda} \mathcal{L}(y, u, \lambda), \chi \rangle = \int_{0}^{T} (\langle \partial_{t} y, \chi \rangle_{V', V} + \int_{\Omega} (\nabla y \cdot \nabla \chi - u \chi) \, d\mathbf{x}) \, dt,$$

which implies that $y \in V$ is the weak solution of the state equation (1.2) (also called the primal problem). Taking the derivative of \mathcal{L} with respect to y and equating this to zero, and obtain for all $\chi \in W(0,T)$

$$0 = \langle \partial_{y} \mathcal{L}(y, u, \lambda), \chi \rangle = \int_{0}^{T} \left(\langle \partial_{t} \chi, \lambda \rangle_{V', V} + \int_{\Omega} \left((y - \hat{y}) \chi + \nabla \chi \cdot \nabla \lambda \right) d\mathbf{x} \right) dt$$
$$= \langle \chi(T), \lambda(T) + \gamma(y(T) - \hat{y}(T)) \rangle_{L^{2}(\Omega)} - \langle \chi(0), \lambda(0) \rangle_{L^{2}(\Omega)}$$
$$+ \int_{0}^{T} \langle -\partial_{t} \lambda - \Delta \lambda + (y - \hat{y}), \chi \rangle_{V', V} dt,$$

where we used integration by parts with respect to t in $\partial_t \chi$ and with respect to \mathbf{x} in $\nabla \chi$. By choosing $\chi \in C_0^{\infty}(Q)$ and applying an argument of density, we find that the last integral is zero. Choosing then $\chi \in W(0,T)$ such that $\chi(0) = 0$, we obtain the adjoint equation (also called the dual problem)

88 (2.1)
$$\begin{aligned} \partial_t \lambda + \Delta \lambda &= y - \hat{y} & \text{in } Q, \\ \lambda &= 0 & \text{on } \Sigma, \\ \lambda(T) &= -\gamma(y(T) - \hat{y}(T)) & \text{on } \Sigma_T := \Omega \times \{T\}. \end{aligned}$$

Finally, taking the derivative of \mathcal{L} with respect to u and equating this to zero, we obtain for all test functions $\chi \in L^2(Q)$, $0 = \langle \partial_u(y, u, p), \chi \rangle = \int_0^T \int_{\Omega} (\nu u - \lambda) \chi \, d\mathbf{x} \, dt$, which gives the optimality condition

92 (2.2)
$$\lambda = \nu u \quad \text{in } Q.$$

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If a control u is optimal with the associated state y of the optimization problem (1.1)-93 (1.2), then the first-order optimality system (1.2), (2.1) and (2.2) must be satisfied. 94 This is a forward-backward system, i.e., the primal problem is solved forward in time 95 with an initial condition while the dual problem is solved backward in time with a 96 final condition, and our new time decomposition algorithms solve this system. Since 97 the time variable plays a special role, we consider a semi-discretization in space, and 98 replace the spatial operator $-\Delta$ in the primal problem (1.2) by a matrix $A \in \mathbb{R}^{n \times n}$, 99 for instance using a Finite Difference discretization in space. We then obtain as above 100 101 the semi-discrete optimality system (dot denoting the time derivative)

$$\begin{cases} \dot{\boldsymbol{y}} + A\boldsymbol{y} = \boldsymbol{u} & \text{in } (0, T), \\ \boldsymbol{y}(0) = \boldsymbol{y}_0, \end{cases} \begin{cases} \dot{\boldsymbol{\lambda}} - A^T \boldsymbol{\lambda} = \boldsymbol{y} - \hat{\boldsymbol{y}} & \text{in } (0, T), \\ \boldsymbol{\lambda}(T) = -\gamma(\boldsymbol{y}(T) - \hat{\boldsymbol{y}}(T)), \end{cases}$$

where $\lambda(t) = \nu u(t)$ for all $t \in \Omega$. Eliminating u, we obtain in matrix form

104 (2.3)
$$\begin{cases} \begin{pmatrix} \dot{\boldsymbol{y}} \\ \dot{\boldsymbol{\lambda}} \end{pmatrix} + \begin{pmatrix} A & -\nu^{-1}I \\ -I & -A^T \end{pmatrix} \begin{pmatrix} \boldsymbol{y} \\ \boldsymbol{\lambda} \end{pmatrix} = \begin{pmatrix} 0 \\ -\hat{\boldsymbol{y}} \end{pmatrix} \text{ in } (0,T), \\ \boldsymbol{y}(0) = \boldsymbol{y}_0, \\ \boldsymbol{\lambda}(T) + \gamma \boldsymbol{y}(T) = \gamma \hat{\boldsymbol{y}}(T), \end{cases}$$

where I is the identity. If A is symmetric, $A = A^T$, which is natural for discretizations of $-\Delta$, then it can be diagonalized, $A = PDP^{-1}$, $D := \text{diag}(d_1, \ldots, d_n)$ with d_i the i-th eigenvalue of A. The system (2.3) can thus also be diagonalized

$$\begin{cases} \begin{pmatrix} \dot{\boldsymbol{z}} \\ \dot{\boldsymbol{\mu}} \end{pmatrix} + \begin{pmatrix} D & -\nu^{-1}I \\ -I & -D \end{pmatrix} \begin{pmatrix} \boldsymbol{z} \\ \boldsymbol{\mu} \end{pmatrix} = \begin{pmatrix} 0 \\ -\hat{\boldsymbol{z}} \end{pmatrix} \text{ in } (0,T), \\ \boldsymbol{z}(0) = \boldsymbol{z}_0, \\ \boldsymbol{\mu}(T) + \gamma \boldsymbol{z}(T) = \gamma \hat{\boldsymbol{z}}(T), \end{cases}$$

where $z := P^{-1}y$, $\mu := P^{-1}\lambda$, $\hat{z} := P^{-1}\hat{y}$ and $z_0 := P^{-1}y_0$. This system then represents n independent 2×2 systems of ODEs of the form

111 (2.4)
$$\begin{cases} \left(\dot{z}_{(i)} \right) + \left(d_i - \nu^{-1} \right) \left(z_{(i)} \right) = \begin{pmatrix} 0 \\ -\hat{z}_{(i)} \end{pmatrix} & \text{in } (0, T), \\ z_{(i)}(0) = z_{(i),0}, \\ \mu_{(i)}(T) + \gamma z_{(i)}(T) = \gamma \hat{z}_{(i)}(T), \end{cases}$$

where $z_{(i)}$, $\mu_{(i)}$, $\hat{z}_{(i)}$ are the *i*-th components of the vectors z, μ , \hat{z} . Isolating the variable in each equation in (2.4), we find the identities

114 (2.5)
$$\mu_{(i)} = \nu(\dot{z}_{(i)} + d_i z_{(i)}), \qquad z_{(i)} = \dot{\mu}_{(i)} - d_i \mu_{(i)} + \hat{z}_{(i)}.$$

We use the identity of z to eliminate μ , and obtain a second-order ODE from (2.4),

$$\begin{cases} \ddot{z}_{(i)} - (d_i^2 + \nu^{-1})z_{(i)} = -\nu^{-1}\hat{z}_{(i)} \text{ in } (0, T), \\ z_{(i)}(0) = z_{(i),0}, \\ \dot{z}_{(i)}(T) + (\nu^{-1}\gamma + d_i)z_{(i)}(T) = \nu^{-1}\gamma\hat{z}_{(i)}(T). \end{cases}$$

Similarly, we can also eliminate z to get

118 (2.7)
$$\begin{cases} \ddot{\mu}_{(i)} - (d_i^2 + \nu^{-1})\mu_{(i)} = -\dot{\hat{z}}_{(i)} - d_i\hat{z}_{(i)} \text{ in } (0, T), \\ \dot{\mu}_{(i)}(0) - d_i\mu_{(i)}(0) = z_{(i),0} - \hat{z}_{(i)}(0), \\ \gamma\dot{\mu}_{(i)}(T) + (1 - \gamma d_i)\mu_{(i)}(T) = 0. \end{cases}$$

119 To simplify the notation in what follows, we define

120 (2.8)
$$\sigma_i := \sqrt{d_i^2 + \nu^{-1}}, \quad \omega_i := \nu^{-1}\gamma + d_i, \quad \beta_i := 1 - \gamma d_i.$$

- In our analysis for the error, \hat{y} will equal zero, which implies $\hat{z} = 0$, and the solution of (2.6) and (2.7) is then
- 123 (2.9) $z_{(i)}(t) \text{ or } \mu_{(i)}(t) = A_i \cosh(\sigma_i t) + B_i \sinh(\sigma_i t),$
- where A_i, B_i are two coefficients.

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- Remark 2.1. Our arguments above work for any diagonalizable matrix A, and thus our results will apply to more general parabolic optimal control problems than the heat equation. Note also that the diagonalization is only a theoretical tool for our convergence analysis, and not needed to run our new time domain decomposition algorithms.
- 3. Dirichlet-Neumann and Neumann-Dirichlet algorithms in time. We 130 now apply Dirichlet-Neumann (DN) and Neumann-Dirichlet (ND) techniques in time 131 to obtain our new time domain decomposition algorithms to solve the system (2.4), 132 and study their convergence. Focusing on the error equations, we set the initial condition $y_0 = 0$ (i.e., $z_0 = 0$) and the target functions $\hat{y} = 0$ (i.e., $\hat{z} = 0$). We 134 135 decompose the time domain $\Omega := (0,T)$ into two non-overlapping time subdomains $\Omega_1 := (0, \alpha)$ and $\Omega_2 := (\alpha, T)$, where α is the interface. We denote by $z_{i,(i)}$ and $\mu_{i,(i)}$ 136 the restriction to Ω_j , j=1,2 of $z_{(i)}$ and $\mu_{(i)}$. Since system (2.4) is a forward-backward 137 system, it appears natural at first sight to keep this property for the decomposed case, 138 as illustrated in Figure 1: we expect to have a final condition for the adjoint state

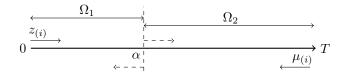


Fig. 1. Illustration of the forward-backward system.

 $\mu_{(i)}$ in Ω_1 since we already have an initial condition for $z_{(i)}$; similarly, we expect to have an initial condition for the primal state $z_{(i)}$ in Ω_2 since we already have a final condition for $\mu_{(i)}$. Therefore, a natural DN algorithm in time solves for the iteration index k = 1, 2, ...

$$\begin{cases} \begin{pmatrix} \dot{z}_{1,(i)}^{k} \\ \dot{\mu}_{1,(i)}^{k} \end{pmatrix} + \begin{pmatrix} d_{i} & -\nu^{-1} \\ -1 & -d_{i} \end{pmatrix} \begin{pmatrix} z_{1,(i)}^{k} \\ \mu_{1,(i)}^{k} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \text{ in } \Omega_{1}, \\ z_{1,(i)}^{k}(0) = 0, \\ \mu_{1,(i)}^{k}(\alpha) = f_{\alpha,(i)}^{k-1}, \\ \begin{pmatrix} \dot{z}_{2,(i)}^{k} \\ \dot{\mu}_{2,(i)}^{k} \end{pmatrix} + \begin{pmatrix} d_{i} & -\nu^{-1} \\ -1 & -d_{i} \end{pmatrix} \begin{pmatrix} z_{2,(i)}^{k} \\ \mu_{2,(i)}^{k} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \text{ in } \Omega_{2}, \\ \dot{z}_{2,(i)}^{k}(\alpha) = \dot{z}_{1,(i)}^{k}(\alpha), \\ \mu_{2,(i)}^{k}(T) + \gamma z_{2,(i)}^{k}(T) = 0, \end{cases}$$

and then the transmission condition is updated by

146 (3.2)
$$f_{\alpha,(i)}^{k} := (1 - \theta) f_{\alpha,(i)}^{k-1} + \theta \mu_{2,(i)}^{k}(\alpha),$$

with a relaxation parameter $\theta \in (0,1)$. However, there are many other ways to decouple in time using DN and ND techniques for problem (2.4): we can apply the technique to both states $(z_{(i)}, \mu_{(i)})$ as in (3.1), or we can apply it just to one of these two states in the reduced forms (2.6) and (2.7). And with the identities (2.5), we can transfer the Dirichlet and the Neumann transmission condition from one state to the other. We list in Table 1 all possible new time domain decomposition algorithms we can obtain, along with their equivalent representations in terms of other formulations. The algorithms can be classified into three main categories, and each category is composed of two blocks, the first block represents a DN technique applied to (2.4), whereas the second block represents a ND technique. Each block contains three rows: the first row is the algorithm applied to formulation (2.4), the second row the algorithm applied to formulation (2.6) and the third row the algorithm applied to formulation (2.7).

Remark 3.1. In Table 1, the transmission conditions $\ddot{z}_{(i)} + d_i \dot{z}_{(i)}$ and $\ddot{\mu}_{(i)} - d_i \dot{\mu}_{(i)}$ are in fact Robin type conditions, since, using the identity (2.5) of $z_{(i)}$ and $\mu_{(i)}$, we find $\dot{z}_{(i)} = \ddot{\mu}_{(i)} - d_i \dot{\mu}_{(i)}$ and $\dot{\mu}_{(i)} = \ddot{z}_{(i)} + d_i \dot{z}_{(i)}$. On the other hand, from the first equation of (2.6) and of (2.7), we have $\ddot{z}_{(i)} - \sigma_i^2 z_{(i)} = 0$ and $\ddot{\mu}_{(i)} - \sigma_i^2 \mu_{(i)} = 0$. Substituting $\ddot{z}_{(i)}$ and $\ddot{\mu}_{(i)}$ gives $\dot{\mu}_{(i)} = \ddot{z}_{(i)} + d_i \dot{z}_{(i)} = d_i \dot{z}_{(i)} + \sigma_i^2 z_{(i)}$ and $\dot{z}_{(i)} = \ddot{\mu}_{(i)} - d_i \dot{\mu}_{(i)} = \sigma_i^2 \mu_{(i)} - d_i \dot{\mu}_{(i)}$. Thus the transmission conditions containing a second derivative in Table 1 are indeed Robin type conditions. We decided to keep the notations $\ddot{z}_{(i)}$ and $\ddot{\mu}_{(i)}$ in Table 1 to show the direct link between the two states $z_{(i)}$ and $\mu_{(i)}$.

 ${\it TABLE~1} \\ {\it Combinations~of~the~DN~and~ND~algorithms.}~ {\it The~letter~R~stands~for~a~Robin~type~condition.}$

	Problem	Ω_1	Ω_2	algorithm type
Category I: $(z_{(i)}, \mu_{(i)})$	(2.4)	$\mu_{(i)}$	$\dot{z}_{(i)}$	(DN)
	(2.6)	$\dot{z}_{(i)} + d_i z_{(i)}$	$\dot{z}_{(i)}$	(RN)
	(2.7)	$\mu_{(i)}$	$\ddot{\mu}_{(i)} - d_i \dot{\mu}_{(i)}$	(DR)
	(2.4)	$\dot{\mu}_{(i)}$	$z_{(i)}$	(ND)
	(2.6)	$\ddot{z}_{(i)} + \dot{d}_i \dot{z}_{(i)}$	$z_{(i)}$	(RD)
	(2.7)	$\dot{\mu}_{(i)}$	$\dot{\mu}_{(i)} - d_i \mu_{(i)}$	(NR)
Category II: $z_{(i)}$	(2.4)	$z_{(i)}$	$\dot{z}_{(i)}$	(DN)
	(2.6)	$z_{(i)}$	$\dot{z}_{(i)}$	(DN)
	(2.7)	$ \dot{\mu}_{(i)} - d_i \mu_{(i)} $	$\ddot{\mu}_{(i)} - \dot{d}_i \dot{\mu}_{(i)}$	(RR)
	(2.4)	$\dot{z}_{(i)}$	$z_{(i)}$	(ND)
	(2.6)	$\dot{z}_{(i)}$	$z_{(i)}$	(ND)
	(2.7)	$\ddot{\mu}_{(i)} - d_i \dot{\mu}_{(i)}$	$\dot{\mu}_{(i)} - d_i \mu_{(i)}$	(RR)
Category III: $\mu_{(i)}$	(2.4)	$\mu_{(i)}$	$\dot{\mu}_{(i)}$	(DN)
	(2.6)	$\dot{z}_{(i)} + \dot{d}_i z_{(i)}$	$\ddot{z}_{(i)} + \dot{d}_i \dot{z}_{(i)}$	(RR)
	(2.7)	$\mu_{(i)}$	$\dot{\mu}_{(i)}$	(DN)
	(2.4)	$\dot{\mu}_{(i)}$	$\mu_{(i)}$	(ND)
	(2.6)	$\ddot{z}_{(i)} + d_i \dot{z}_{(i)}$	$\dot{z}_{(i)} + d_i z_{(i)}$	(RR)
	(2.7)	$\dot{\mu}_{(i)}$	$\mu_{(i)}$	(ND)

However, there are other interpretations of some transmission conditions in certain circumstances. For instance, let us take the Neumann condition $\dot{z}_{(i)}$ in the second block of Category II for the problem (2.4), it can also be interpreted as a Robin condition $\sigma_i^2 \mu_{(i)} - d_i \dot{\mu}_{(i)}$ using the above argument. Then, this algorithm can also be read as a Robin-Dirichlet (RD) type algorithm instead of a Neumann-Dirichlet type. Moreover, this interpretation is particularly useful in this case, since it reveals the fact that the forward-backward property of the problem (2.4) is still kept by this algorithm. Otherwise, we can also use the identity of $\mu_{(i)}$ in (2.5) to transfer this Neumann condition $\dot{z}_{(i)}$ to $\mu_{(i)} - d_i z_{(i)}$. This is also useful from a numerical point of view, since we can transfer a Neumann condition to a Dirichlet type condition. This will be used in detail in the following analysis.

- **3.1. Category I.** We start with the algorithms in Category I, which run on the pair $(z_{(i)}, \mu_{(i)})$ to solve (2.4), and study the DN and then the ND variant.
- **3.1.1. Dirichlet-Neumann algorithm (DN**₁). This is (3.1), at first sight the most natural method that keeps the forward-backward structure as in the original problem (2.4). To analyze the convergence behavior, we can choose any of the problem formulations (2.6), (2.7), since they are equivalent to (2.4). Choosing (2.6), the algorithm DN_1 for i = 1, ..., n, and iteration k = 1, 2, ... is given by

$$\begin{cases} \ddot{z}_{1,(i)}^k - \sigma_i^2 z_{1,(i)}^k = 0 \text{ in } \Omega_1, \\ z_{1,(i)}^k(0) = 0, \\ \dot{z}_{1,(i)}^k(\alpha) + d_i z_{1,(i)}^k(\alpha) = f_{\alpha,(i)}^{k-1}, \end{cases} \begin{cases} \ddot{z}_{2,(i)}^k - \sigma_i^2 z_{2,(i)}^k = 0 \text{ in } \Omega_2, \\ \dot{z}_{2,(i)}^k(\alpha) = \dot{z}_{1,(i)}^k(\alpha), \\ \dot{z}_{2,(i)}^k(T) + \omega_i z_{2,(i)}^k(T) = 0, \end{cases}$$

and the update of the transmission condition defined in (3.2) becomes

188 (3.4)
$$f_{\alpha,(i)}^{k} = (1-\theta)f_{\alpha,(i)}^{k-1} + \theta(\dot{z}_{2,(i)}^{k}(\alpha) + d_{i}z_{2,(i)}^{k}(\alpha)).$$

This is a Robin-Neumann type algorithm applied to solve the problem (2.6). Using 189 the general solution (2.9), and the initial and final condition, we find 190

191 (3.5)
$$z_{1,(i)}^k(t) = A_i^k \sinh(\sigma_i t), \ z_{2,(i)}^k(t) = B_i^k \left(\sigma_i \cosh\left(\sigma_i (T-t)\right) + \omega_i \sinh\left(\sigma_i (T-t)\right)\right),$$

where A_i^k and B_i^k are determined by the transmission conditions at α in (3.3). Note 192

that we will use (3.5) in the analysis for all algorithms, since only the transmission con-193

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that we will use (3.5) in the analysis for an algorithms, since only the transmission confidence of the transmission condition (3.3) and solving for
$$A_i^k$$
, B_i^k gives $A_i^k = \frac{f_{\alpha,(i)}^{k-1}}{\sigma_i \cosh(a_i) + d_i \sinh(a_i)}$ and $B_i^k = \frac{-f_{\alpha,(i)}^{k-1} \cosh(a_i)}{(\sigma_i \cosh(a_i) + d_i \sinh(a_i))(\sigma_i \sinh(b_i) + \omega_i \cosh(b_i))}$, where we let $a_i := \sigma_i \alpha$ and $b_i := \sigma_i (T - \alpha)$ to simplify the notations, and $a_i + b_i = \sigma_i T$.

197 Using the update of the transmission condition (3.4), we obtain $f_{\alpha,(i)}^k = (1 - \theta) f_{\alpha,(i)}^{k-1} + \theta f_{\alpha,(i)}^{k-1} \nu^{-1} \frac{\sigma_i \gamma + \beta_i \tanh(b_i)}{(\sigma_i + d_i \tanh(a_i))(\omega_i + \sigma_i \tanh(b_i))}$, which leads to the following result.

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Theorem 3.2. The algorithm DN_1 (3.1)-(3.2) converges if and only if 199

200 (3.6)
$$\rho_{DN_1} := \max_{d_i \in \lambda(A)} \left| 1 - \theta \left(1 - \nu^{-1} \frac{\sigma_i \gamma + \beta_i \tanh(b_i)}{\left(\sigma_i + d_i \tanh(a_i) \right) \left(\omega_i + \sigma_i \tanh(b_i) \right)} \right) \right| < 1,$$

where $\lambda(A)$ is the spectrum of the matrix A. 201

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Remark 3.3. Instead of focusing on the state $z_{(i)}$ for the analysis, we could also 202 have focused on the state $\mu_{(i)}$, which gives the same result, see Appendix A. 203

To get more insight in the convergence behavior, we consider a few special cases. 204

205 COROLLARY 3.4. If the matrix A is not singular, then the algorithm DN_1 (3.1)-(3.2) for $\theta = 1$ converges for all initial guesses. 206

Proof. Substituting $\theta = 1$ into (3.6), we have

208 (3.7)
$$\rho_{\mathrm{DN}_1}|_{\theta=1} = \nu^{-1} \max_{d_i \in \lambda(A)} \left| \frac{\sigma_i \gamma + \beta_i \tanh(b_i)}{\left(\sigma_i + d_i \tanh(a_i)\right) \left(\omega_i + \sigma_i \tanh(b_i)\right)} \right|.$$

Using the definition of σ_i , β_i and ω_i from (2.8), the numerator can be written as $\sigma_i \gamma +$ 209

 $\beta_i \tanh(b_i) = \gamma(\sigma_i - d_i \tanh(b_i)) + \tanh(b_i)$. Since $0 < \tanh(x) < 1, \forall x > 0$ and $\sigma_i - d_i \tanh(b_i) = \gamma(\sigma_i - d_i \tanh(b_i))$ 210

 $d_i \tanh(b_i) > 0$, both the numerator and the denominator in (3.7) are positive. Now

the difference between the numerator and the denominator is $(\sigma_i + d_i \tanh(a_i))(\omega_i +$

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 $\sigma_{i} \tanh(b_{i}) - \nu^{-1}(\sigma_{i}\gamma + \beta_{i} \tanh(b_{i})) = (1 + \tanh(b_{i}) \tanh(a_{i}))(\sigma_{i}d_{i} + \omega_{i}d_{i} \tanh(\sigma_{i}T)) > 0, \text{ meaning that for each eigenvalue } d_{i}, 0 < \nu^{-1} \frac{\sigma_{i}\gamma + \beta_{i} \tanh(b_{i})}{(\sigma_{i} + d_{i} \tanh(a_{i}))(\omega_{i} + \sigma_{i} \tanh(b_{i}))} < 1. \quad \Box$ 214

Remark 3.5. For the Laplace operator with homogeneous Dirichlet boundary con-215

ditions in our model problem (1.2), there is no zero eigenvalue for its discretization

matrix A. If an eigenvalue $d_i = 0$, we have $\sigma_i|_{d_i=0} = \sqrt{\nu^{-1}}$, $\omega_i|_{d_i=0} = \gamma \nu^{-1}$ and 217 $\beta_i|_{d_i=0}=1$. Substituting these values into the convergence factor (3.7), we find

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 $\rho_{\mathrm{DN}_1}|_{\theta=1,d_i=0} = \nu^{-1} \frac{\sqrt{\nu^{-1}}\gamma + \tanh(\sqrt{\nu^{-1}}(T-\alpha))}{\sqrt{\nu^{-1}}(\gamma\nu^{-1}+\sqrt{\nu^{-1}}\tanh(\sqrt{\nu^{-1}}(T-\alpha)))} = 1$, and convergence is lost. The convergence behavior of the algorithm DN_1 for small eigenvalues is thus not 219

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good. Furthermore, inserting $d_i = 0$ into (3.6) and using the above result, we find 221

that $\rho_{\text{DN}_1}|_{d_i=0}=1$, independently of the relaxation parameter θ and the interface 222 position α : relaxation can not fix this problem. 223

Remark 3.6. If some d_i goes to infinity, we have $\sigma_i \sim_{\infty} d_i$ and $\omega_i \sim_{\infty} d_i$, and therefore $\lim_{d_i \to \infty} \left| 1 - \theta \left(1 - \nu^{-1} \frac{\sigma_i \gamma + \beta_i \tanh(b_i)}{(\sigma_i + d_i \tanh(a_i))(\omega_i + \sigma_i \tanh(b_i))} \right) \right| = |1 - \theta|$, which is independent of α , so high frequency convergence is robust with relaxation. One can 224 225

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use $\theta = 1$ to get a good smoother, with the following convergence factor estimate. 227

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COROLLARY 3.7. If A is positive semi-definite, then the algorithm DN_1 (3.1)-229 (3.2) with $\theta = 1$ satisfies the convergence estimate $\rho_{DN_1}|_{\theta=1} \leq \frac{1+\gamma\sigma_{\min}}{\nu d_{\min}^2}$, with $d_{\min} := \min \lambda(A)$ the smallest eigenvalue of A.

231 Proof. Since for $\theta=1$, Corollary 3.4 shows that the convergence factor is between 232 0 and 1 for each eigenvalue d_i , we can take (3.7) and remove the absolute value, 233 $\rho_{\mathrm{DN}_1}|_{\theta=1}=\nu^{-1}\max_{d_i\in\lambda(A)}\frac{\tanh(b_i)+\gamma(\sigma_i-d_i\tanh(b_i))}{(\sigma_i+d_i\tanh(a_i))(\omega_i+\sigma_i\tanh(b_i))}$. Using the definition of σ_i 234 and ω_i from (2.8), we have $\sigma_i>d_i\geq 0$ and $\omega_i\geq d_i\geq 0$. Since $0<\tanh(x)<1$, $\forall x>0$, we obtain that $\sigma_i+d_i\tanh(a_i)\geq d_i$, $\omega_i+\sigma_i\tanh(b_i)\geq d_i$ and $\sigma_i-d_i\tanh(b_i)\leq \sigma_i$. 236 This implies $\frac{\tanh(b_i)+\gamma(\sigma_i-d_i\tanh(b_i))}{(\sigma_i+d_i\tanh(a_i))(\omega_i+\sigma_i\tanh(b_i))}\leq \frac{1+\gamma\sigma_i}{d_i^2}=\frac{1}{d_i}(\frac{1}{d_i}+\gamma\frac{\sigma_i}{d_i})$. Using once again 237 the definition of σ_i from (2.8), we find $\frac{\sigma_i}{d_i}=\sqrt{1+\frac{\nu^{-1}}{d_i^2}}\leq \sqrt{1+\frac{\nu^{-1}}{d_{\min}^2}}$. Hence, we have 238 $\frac{1+\gamma\sigma_i}{d_i^2}\leq \frac{1+\gamma\sigma_{\min}}{d_{\min}^2}$, which concludes the proof.

Since A comes from a spatial discretization, the smallest eigenvalue of A depends only little on the spatial mesh size, and convergence is thus robust under mesh refinement. Corollary 3.7 is however less useful when ν is small: for example for $\gamma=0$, the bound is less than one only if $\nu>\frac{1}{d_{\min}^2}$, but we have also the following convergence result.

Theorem 3.8. The algorithm DN_1 (3.1)-(3.2) converges for all initial guesses under the assumption that the matrix A is not singular.

Proof. From Corollary 3.4, we know that the convergence factor satisfies $0 < \rho_{\mathrm{DN}_1}|_{\theta=1} < 1$. Using its definition (3.6), we find for $\theta \in (0,1)$, $0 < 1 - \theta < \rho_{\mathrm{DN}_1} = 1 - \theta(1 - \rho_{\mathrm{DN}_1}|_{\theta=1}) < 1$, which concludes the proof.

Remark 3.9. As shown in the previous proof, the function $g(\theta) := 1 - \theta(1 - \rho_{\mathrm{DN}_1}|_{\theta=1})$ is decreasing for $\theta \in (0,1)$, which makes $\theta=1$ the best relaxation parameter. This is further confirmed by our numerical experiments (see Figure 4). Due to the bad convergence behavior of the algorithm DN_1 for small eigenvalues, it only makes this most natural DN algorithm a good smoother but not a good solver.

3.1.2. Neumann-Dirichlet algorithm (ND₁). We now invert the two conditions, and apply the Neumann condition to the state $\mu_{(i)}$ in Ω_1 and the Dirichlet condition to the state $z_{(i)}$ in Ω_2 , still respecting the forward-backward structure. For iteration index $k = 1, 2, \ldots$, the algorithm ND₁ computes

$$\begin{cases} \left(\dot{z}_{1,(i)}^{k}\right) + \left(d_{i} - \nu^{-1}\right) \begin{pmatrix} z_{1,(i)}^{k} \\ \mu_{1,(i)}^{k} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \text{ in } \Omega_{1}, \\ z_{1,(i)}^{k}(0) = 0, \\ \dot{\mu}_{1,(i)}^{k}(\alpha) = \dot{\mu}_{2,(i)}^{k}(\alpha), \\ \left(\dot{z}_{2,(i)}^{k} \\ \dot{\mu}_{2,(i)}^{k} \end{pmatrix} + \left(d_{i} - \nu^{-1} \\ -1 - d_{i} \right) \begin{pmatrix} z_{2,(i)}^{k} \\ \mu_{2,(i)}^{k} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \text{ in } \Omega_{2}, \\ z_{2,(i)}^{k}(\alpha) = f_{\alpha,(i)}^{k-1}, \\ \mu_{2,(i)}^{k}(T) + \gamma z_{2,(i)}^{k}(T) = 0, \end{cases}$$

258 and we update the transmission condition by

259 (3.9)
$$f_{\alpha,(i)}^k := (1 - \theta) f_{\alpha,(i)}^{k-1} + \theta z_{1,(i)}^k(\alpha), \quad \theta \in (0, 1).$$

260 For the convergence analysis, we choose to use the formulation (2.7), i.e.

$$\begin{cases}
\ddot{\mu}_{1,(i)}^{k} - \sigma_{i}^{2} \mu_{1,(i)}^{k} = 0 \text{ in } \Omega_{1}, \\
\dot{\mu}_{(i)}(0) - d_{i} \mu_{(i)}(0) = 0, \\
\dot{\mu}_{1,(i)}^{k}(\alpha) = \dot{\mu}_{2,(i)}^{k}(\alpha),
\end{cases}
\begin{cases}
\ddot{\mu}_{2,(i)}^{k} - \sigma_{i}^{2} \mu_{2,(i)}^{k} = 0 \text{ in } \Omega_{2}, \\
\dot{\mu}_{2,(i)}^{k}(\alpha) - d_{i} \mu_{2,(i)}^{k}(\alpha) = f_{\alpha,(i)}^{k-1}, \\
\gamma \dot{\mu}_{(i)}(T) + \beta_{i} \mu_{(i)}(T) = 0,
\end{cases}$$

where the update of the transmission condition (3.9) becomes 262

263 (3.11)
$$f_{\alpha,(i)}^{k} = (1 - \theta) f_{\alpha,(i)}^{k-1} + \theta \left(\dot{\mu}_{1,(i)}^{k}(\alpha) - d_{i} \mu_{1,(i)}^{k}(\alpha) \right), \quad \theta \in (0,1).$$

- The algorithm ND_1 (3.8) can thus be interpreted as a NR type algorithm (3.10). 264
- Using the general solution (2.9) and the initial and final conditions, we get 265

$$\mu_{1,(i)}^{k}(t) = A_{i}^{k} \left(\sigma_{i} \cosh(\sigma_{i}t) + d_{i} \sinh(\sigma_{i}t) \right),$$

$$\mu_{2,(i)}^{k}(t) = B_{i}^{k} \left(\gamma \sigma_{i} \cosh\left(\sigma_{i}(T-t)\right) + \beta_{i} \sinh\left(\sigma_{i}(T-t)\right) \right),$$

- and from the transmission condition in (3.10) on each domain, and we obtain $A_i^k = \frac{f_{\alpha,(i)}^{k-1}(\sigma_i\gamma\sinh(b_i)+\beta_i\cosh(b_i))}{(\omega_i\sinh(b_i)+\sigma_i\cosh(b_i))(\sigma_i\sinh(a_i)+d_i\cosh(a_i))}$ and $B_i^k = \frac{-f_{\alpha,(i)}^{k-1}}{\omega_i\sinh(b_i)+\sigma_i\cosh(b_i)}$. Using the relation (3.11), we find $f_{\alpha,(i)}^k = (1-\theta)f_{\alpha,(i)}^{k-1} + \theta f_{\alpha,(i)}^{k-1} \nu^{-1} \frac{\sigma_i\gamma+\beta_i\coth(b_i)}{(\sigma_i+d_i\coth(a_i))(\omega_i+\sigma_i\coth(b_i))}$, 267
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- which leads to the following result. 270

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THEOREM 3.10. The algorithm ND_1 (3.8)-(3.9) converges if and only if 271

272 (3.13)
$$\rho_{ND_1} := \max_{d_i \in \lambda(A)} \left| 1 - \theta \left(1 - \nu^{-1} \frac{\sigma_i \gamma + \beta_i \coth(b_i)}{\left(\sigma_i + d_i \coth(a_i) \right) \left(\omega_i + \sigma_i \coth(b_i) \right)} \right) \right| < 1.$$

- The convergence factor of the algorithm ND_1 (3.13) is very similar to that of DN_1 (3.6). 273
- For instance, the behavior for large and small eigenvalues shown in Remarks 3.5 and 274
- 3.6 still hold: when inserting $d_i=0$ into (3.13) we find $\rho_{\mathrm{ND}_1}|_{d_i=0}=|1-\theta(1-\theta)|_{d_i=0}$ 275
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- so still hold. When inserting $d_i = 0$ into (3.15) we find $p_{\text{ND}_1}|d_i = 0 = |1 \nu(1 \nu^{-1} \frac{\sqrt{\nu^{-1}}\gamma + \coth(\sqrt{\nu^{-1}}(T-\alpha))}{\sqrt{\nu^{-1}}(\gamma\nu^{-1} + \sqrt{\nu^{-1}}\cot(\sqrt{\nu^{-1}}(T-\alpha)))})| = 1$, again independent of the relaxation parameter θ and the interface position α ; and when the eigenvalue d_i goes to infinity, we find $\lim_{d_i \to \infty} |1 \theta(1 \nu^{-1} \frac{\sigma_i \gamma + \beta_i \cot(b_i)}{(\sigma_i + d_i \cot(a_i))(\omega_i + \sigma_i \cot(b_i))})| = |1 \theta|$, again independent of the interface position α . Due however to the presence of the hyperbolic cotangent 278
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- function in (3.13) instead of the hyperbolic tangent function in (3.6), we need further 280 assumptions to obtain results like Corollaries 3.4 and 3.7. Indeed, substituting $\theta = 1$ 281
- 282 into (3.13) and using the definition of σ_i , β_i from (2.8), the numerator reads $\sigma_i \gamma$ +
- $\beta_i \coth(b_i) = \gamma(\sqrt{d_i^2 + \nu^{-1}} d_i \coth(\sqrt{d_i^2 + \nu^{-1}}(T \alpha))) + \coth(\sqrt{d_i^2 + \nu^{-1}}(T \alpha)).$ 283
- Depending on γ, ν and α , this value could be negative. However, by setting $\gamma = 0$, 284
- the numerator is guaranteed to be positive, and we obtain the following results. 285
- COROLLARY 3.11. If A is not singular and the parameter $\gamma = 0$, then the algo-286 rithm ND_1 (3.8)-(3.9) for $\theta = 1$ converges for all initial guesses. 287
 - *Proof.* Substituting $\theta = 1$ and $\gamma = 0$ into (3.13), we get

289 (3.14)
$$\rho_{\text{ND}_2}|_{\theta=1} = \nu^{-1} \max_{d_i \in \lambda(A)} \left| \frac{\coth(b_i)}{(\sigma_i + d_i \coth(a_i))(d_i + \sigma_i \coth(b_i))} \right|.$$

- Since $\coth(x) > 1$, $\forall x > 0$, both the numerator and the denominator in (3.14) are 290
- positive, and the difference between them is $(\sigma_i + d_i \coth(a_i))(d_i + \sigma_i \coth(b_i))$ –
- $\nu^{-1} \coth(b_i) = (\coth(a_i) + \coth(b_i))(d_i^2 + \sigma_i d_i \coth(\sigma_i T)) > 0$, meaning that for each eigenvalue d_i , $0 < \nu^{-1} \frac{\coth(b_i)}{(\sigma_i + d_i \coth(a_i))(\omega_i + \sigma_i \coth(b_i))} < 1$, which concludes the proof. \square

COROLLARY 3.12. If A is positive semi-definite and the parameter $\gamma = 0$, then the algorithm ND₁ (3.8)-(3.9) for $\theta = 1$ satisfies the convergence estimate

296 (3.15)
$$\rho_{ND_1}|_{\theta=1} \le \frac{\coth\left(\sigma_{\min}(T-\alpha)\right)}{\nu(\sigma_{\min}+d_{\min})^2}.$$

297 Proof. Since we have shown in Corollary 3.11 that the convergence factor is between 0 and 1 for each eigenvalue d_i , we can take (3.14) and remove the absolute value, $\rho_{\text{ND}_2}|_{\theta=1} = \nu^{-1} \max_{d_i \in \lambda(A)} \frac{\coth(b_i)}{(\sigma_i + d_i \coth(a_i))(d_i + \sigma_i \coth(b_i))}$. Since $\sigma_i = \sqrt{d_i^2 + \nu^{-1}} \geq 0$ and $\cot(x) > 1$, $\forall x > 0$, we obtain that $\sigma_i + d_i \coth(a_i) \geq \sigma_i + d_i$ and $d_i + \sigma_i \coth(b_i) \geq \sigma_i + d_i$. This implies that $\frac{\coth(b_i)}{(\sigma_i + d_i \coth(a_i))(d_i + \sigma_i \coth(b_i))} \leq \frac{\coth(b_i)}{(\sigma_i + d_i)^2}$. Recalling $\coth(b_i) = \coth(\sigma_i(T - \alpha))$, and using the fact that $d_i \geq d_{\min}$ and $\sigma_i \geq 0$ and $\sigma_i = \sqrt{d_{\min}^2 + \nu^{-1}}$, we find $\frac{\coth(b_i)}{(\sigma_i + d_i)^2} \leq \frac{\coth(\sigma_{\min}(T - \alpha))}{(\sigma_{\min} + d_{\min})^2}$, which concludes the proof.

Like for DN₁, the estimate (3.15) is independent of the spatial mesh size, and since for $\gamma = 0$, the convergence factor satisfies $0 < \rho_{\text{ND}_1}|_{\theta=1} < 1$ as shown in Corollary 3.11, using the definition of the convergence factor (3.13), we obtain the following result.

Theorem 3.13. The algorithm ND_1 (3.8)-(3.9) converges for all initial guesses if $\gamma = 0$ and the matrix A is not singular.

- 309 **3.2. Category II.** We now study algorithms in Category II which run only on the state $z_{(i)}$ to solve the problem (2.4), based on DN and ND techniques.
- 3.2.1. Dirichlet-Neumann algorithm (DN₂). As explained in Table 1, we apply the Dirichlet condition in Ω_1 and the Neumann condition in Ω_2 both on the primal state $z_{(i)}$. For the iteration index k = 1, 2, ..., the algorithm DN₂ solves

$$\begin{cases} \begin{pmatrix} \dot{z}_{1,(i)}^{k} \\ \dot{\mu}_{1,(i)}^{k} \end{pmatrix} + \begin{pmatrix} d_{i} & -\nu^{-1} \\ -1 & -d_{i} \end{pmatrix} \begin{pmatrix} z_{1,(i)}^{k} \\ \mu_{1,(i)}^{k} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \text{ in } \Omega_{1}, \\ z_{1,(i)}^{k}(0) = 0, \\ z_{1,(i)}^{k}(\alpha) = f_{\alpha,(i)}^{k-1}, \\ \begin{pmatrix} \dot{z}_{2,(i)}^{k} \\ \dot{\mu}_{2,(i)}^{k} \end{pmatrix} + \begin{pmatrix} d_{i} & -\nu^{-1} \\ -1 & -d_{i} \end{pmatrix} \begin{pmatrix} z_{2,(i)}^{k} \\ \mu_{2,(i)}^{k} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \text{ in } \Omega_{2}, \\ \dot{z}_{2,(i)}^{k}(\alpha) = \dot{z}_{1,(i)}^{k}(\alpha), \\ \mu_{2,(i)}^{k}(T) + \gamma z_{2,(i)}^{k}(T) = 0, \end{cases}$$

and we update the transmission condition by

316 (3.17)
$$f_{\alpha,(i)}^k := (1 - \theta) f_{\alpha,(i)}^{k-1} + \theta z_{2,(i)}^k(\alpha), \quad \theta \in (0,1).$$

At first glance, this algorithm does not have the forward-backward structure, with both an initial and a final condition on $z_{1,(i)}$ in Ω_1 and nothing on $\mu_{1,(i)}$. However, as mentioned in Remark 3.1, this is only a matter of interpretation: using the identity of $z_{(i)}$ from (2.5), we can rewrite the transmission condition $z_{1,(i)}^k(\alpha) = f_{\alpha,(i)}^{k-1}$ as $\dot{\mu}_{1,(i)}^k(\alpha) - d_i \mu_{1,(i)}^k(\alpha) = f_{\alpha,(i)}^{k-1}$, and define the update (3.17) as $f_{\alpha,(i)}^k := (1-\theta) f_{\alpha,(i)}^{k-1} + \theta(\dot{\mu}_{2,(i)}^k(\alpha) - d_i \mu_{2,(i)}^k(\alpha))$, to rediscover the forward-backward structure. Moreover, with the interpretation of $\mu_{1,(i)}^k$, the algorithm DN₂ (3.16) is a RN type algorithm.

For the analysis, we choose the state $z_{(i)}$ formulation: for i = 1, ..., n and iteration 324 325 index $k = 1, 2, \ldots$, the equivalent algorithm reads

$$\begin{cases} \ddot{z}_{1,(i)}^{k} - \sigma_{i}^{2} z_{1,(i)}^{k} = 0 \text{ in } \Omega_{1}, \\ z_{1,(i)}^{k}(0) = 0, \\ z_{1,(i)}^{k}(\alpha) = f_{\alpha,(i)}^{k-1}, \end{cases} \begin{cases} \ddot{z}_{2,(i)}^{k} - \sigma_{i}^{2} z_{2,(i)}^{k} = 0 \text{ in } \Omega_{2}, \\ \dot{z}_{2,(i)}^{k}(\alpha) = \dot{z}_{1,(i)}^{k}(\alpha), \\ \dot{z}_{2,(i)}^{k}(T) + \omega_{i} z_{2,(i)}^{k}(T) = 0, \end{cases}$$

- where we still update the transmission condition by (3.17). Note that (3.18) is still a 327
- DN type algorithm, like (3.16). Using the solutions (3.5) to determine the two coef-328
- ficients A_i^k and B_i^k , we get from (3.18) $A_i^k = \frac{f_{\alpha,(i)}^{k-1}}{\sinh(a_i)}$ and $B_i^k = -\frac{f_{\alpha,(i)}^{k-1}\coth(a_i)}{\sigma_i\sinh(b_i)+\omega_i\cosh(b_i)}$. With (3.17), we find $f_{\alpha,(i)}^k = (1-\theta)f_{\alpha,(i)}^{k-1} \theta f_{\alpha,(i)}^{k-1}\coth(a_i)\frac{\sigma_i\cosh(b_i)+\omega_i\sinh(b_i)}{\sigma_i\sinh(b_i)+\omega_i\cosh(b_i)}$, and 329
- 330
- thus obtain the following convergence results. 331
- Theorem 3.14. The algorithm DN_2 (3.16)-(3.17) converges if and only if 332

333 (3.19)
$$\rho_{DN_2} := \max_{d_i \in \lambda(A)} \left| 1 - \theta \left(1 + \coth(a_i) \frac{\sigma_i \coth(b_i) + \omega_i}{\sigma_i + \omega_i \coth(b_i)} \right) \right| < 1.$$

- COROLLARY 3.15. The algorithm DN_2 for $\theta = 1$ does not converge if $\alpha \leq \frac{T}{2}$. 334
- *Proof.* Substituting $\theta = 1$ into (3.19), we have 335

336 (3.20)
$$\rho_{\mathrm{DN}_2}|_{\theta=1} = \max_{d_i \in \lambda(A)} \left| \coth(a_i) \frac{\sigma_i \coth(b_i) + \omega_i}{\sigma_i + \omega_i \coth(b_i)} \right|.$$

- Since $\coth(x) > 1$, $\forall x > 0$, both the numerator and the denominator in (3.20) are 337
- positive. When $a_i \leq b_i$ (i.e., $\alpha \leq T \alpha$), we have $\coth(a_i) \geq \coth(b_i)$, and thus the 338
- difference between the numerator and the denominator is $\coth(a_i)(\omega_i + \sigma_i \coth(b_i))$ 339
- $(\sigma_i + \omega_i \coth(b_i)) = \omega_i(\coth(a_i) \coth(b_i)) + \sigma_i(\coth(b_i) \coth(a_i) 1) > 0, \text{ meaning that } \coth(a_i) \frac{\sigma_i \coth(b_i) + \omega_i}{\sigma_i + \omega_i \coth(b_i)} > 1, \text{ which concludes the proof.}$ 340
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- We need some extra assumptions to conclude for the case $\alpha > \frac{T}{2}$. 342
- COROLLARY 3.16. The algorithm DN_2 for $\theta = 1$ does not converge if $\gamma = 0$. 343
- *Proof.* We showed in Corollary 3.15 the result for $\alpha \leq \frac{T}{2}$. Now $\alpha > \frac{T}{2}$ implies that $a_i > b_i$, thus $\coth(a_i) < \coth(b_i)$. Inserting $\gamma = 0$ into (3.20) and using the definition 344 345
- of σ_i from (2.8), the difference between the numerator and the denominator of (3.20) 346
- becomes $\coth(a_i)(d_i + \sigma_i \coth(b_i)) (\sigma_i + d_i \coth(b_i)) = (\coth(a_i) \coth(b_i))(d_i + d_i \coth(b_i))$ 347
- $\sigma_i \coth(b_i a_i) > 0$, where we use the fact that $d_i + \sigma_i \coth(b_i a_i) < d_i \sigma_i < 0$. This shows that DN₂ for $\theta = 1$ also does not converge for $\alpha > \frac{T}{2}$ when $\gamma = 0$. 348
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- Unlike in Corollary 3.7 where we have an estimate of the convergence factor for 350
- DN_1 , we cannot provide a general convergence estimate for the algorithm DN_2 (3.16)-351
- (3.17), since we showed in Corollary 3.15 and Corollary 3.16 that it does not converge 352
- 353 in some cases. However, we can still show the convergence behavior for extreme
- eigenvalues. In particular, if the eigenvalue $d_i = 0$, we find 354

355 (3.21)
$$\rho_{\mathrm{DN}_2}|_{d_i=0} = \left| 1 - \theta \left(1 + \coth(\sqrt{\nu^{-1}}\alpha) \frac{\coth\left(\sqrt{\nu^{-1}}(T-\alpha)\right) + \gamma\sqrt{\nu^{-1}}}{1 + \gamma\sqrt{\nu^{-1}}\coth\left(\sqrt{\nu^{-1}}(T-\alpha)\right)} \right) \right|.$$

When the eigenvalue goes to infinity, using Remark 3.6, we obtain $\lim_{d_i \to \infty} \rho_{DN_2} =$ 356 $|1-2\theta|$. By equioscillating the convergence factor for small (i.e., $\rho_{\mathrm{DN}_2}|_{d_i=0}$) and large 357

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358 eigenvalues (i.e., $\rho_{\mathrm{DN}_2}|_{d_i\to\infty}$), we obtain after some computations

$$\theta_{\mathrm{DN}_2}^* = \frac{2}{3 + \coth(\sqrt{\nu^{-1}}\alpha) \frac{\coth(\sqrt{\nu^{-1}}(T-\alpha)) + \gamma\sqrt{\nu^{-1}}}{1 + \gamma\sqrt{\nu^{-1}}\coth(\sqrt{\nu^{-1}}(T-\alpha))}}.$$

THEOREM 3.17. If we assume that the eigenvalues of A are anywhere in the inter-360 val $[0,\infty)$, then the optimal relaxation parameter $\theta_{DN_2}^{\star}$ for the algorithm DN_2 (3.16)-361 (3.17) with $\gamma = 0$ is given by (3.22) and satisfies $\theta_{DN_2}^{\star} < \frac{1}{2}$. 362

Proof. Taking the derivative of the convergence factor ρ_{DN_2} from (3.19) with respect to the eigenvalue d_i , we get $\frac{\mathrm{d}\rho_{\text{DN}_2}}{\mathrm{d}d_i} = -\frac{d_i\alpha}{\sigma_i\sinh^2(a_i)}\frac{\sigma_i\coth(b_i)+\omega_i}{\sigma_i+\omega_i\coth(b_i)} - \frac{\nu^{-1}\coth(a_i)}{\sigma_i}$ 364 $\frac{\beta_i(\coth^2(b_i)-1) + \frac{d_i(T-\alpha)}{\sinh^2(b_i)}(1-\gamma^2\nu^{-1}-2d_i\gamma)}{(\sigma_i + \omega_i \coth(b_i))^2}, \text{ where we used } \sigma_i, \omega_i \text{ and } \beta_i \text{ from (2.8)}. \text{ The de-}$

rivative becomes negative with $\gamma = 0$, meaning that the convergence factor decreases 366 with respect to the eigenvalue d_i . We can then deduce the optimal relaxation pa-367 rameter using equioscillation: inserting $\gamma = 0$ into (3.22), the denominator becomes 368 $3 + \coth(\sqrt{\nu^{-1}}\alpha) \coth(\sqrt{\nu^{-1}}(T - \alpha)) < 4.$ 369

For $\gamma > 0$, it is not clear when the convergence factor $\rho_{\rm DN_2}$ is monotonic with 370 respect to the eigenvalues, and thus the optimal relaxation parameter $\theta_{\rm DN_2}^{\star}$ could 371 differ from (3.22). 372

3.2.2. Neumann-Dirichlet algorithm (ND_2) . We now invert the two condi-373 tions: for the iteration index k = 1, 2, ..., the algorithm ND₂ to study is 374

$$\begin{cases} \left(\dot{z}_{1,(i)}^{k}\right) + \left(d_{i} - \nu^{-1}\right) \begin{pmatrix} z_{1,(i)}^{k} \\ \mu_{1,(i)}^{k} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \text{ in } \Omega_{1}, \\ z_{1,(i)}^{k}(0) = 0, \\ \dot{z}_{1,(i)}^{k}(\alpha) = f_{\alpha,(i)}^{k-1}, \\ \left(\dot{z}_{2,(i)}^{k} \\ \dot{\mu}_{2,(i)}^{k} \end{pmatrix} + \begin{pmatrix} d_{i} - \nu^{-1} \\ -1 - d_{i} \end{pmatrix} \begin{pmatrix} z_{2,(i)}^{k} \\ \mu_{2,(i)}^{k} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \text{ in } \Omega_{2}, \\ z_{2,(i)}^{k}(\alpha) = z_{1,(i)}^{k}(\alpha), \\ \mu_{2,(i)}^{k}(T) + \gamma z_{2,(i)}^{k}(T) = 0, \end{cases}$$

and then we update the transmission condition by 376

377 (3.24)
$$f_{\alpha,(i)}^k := (1 - \theta) f_{\alpha,(i)}^{k-1} + \theta \dot{z}_{2,(i)}^k(\alpha), \quad \theta \in (0,1).$$

Similar to the algorithm DN₂ (3.16)-(3.17), we cannot see the forward-backward struc-378 ture in Ω_1 for the algorithm ND₂ (3.23)-(3.24). But by interpreting the Neumann con-379 dition on $z_{1,(i)}$ in terms of $\mu_{1,(i)}$ as explained in Remark 3.1, the forward-backward 380 structure is again revealed through a RD type algorithm. 381

382 We proceed for the convergence analysis using the formulation (2.6): for i = $1, \ldots, n$ and iteration index $k = 1, 2, \ldots$, we solve 383

$$\begin{cases}
\ddot{z}_{1,(i)}^{k} - (d_{i}^{2} + \nu^{-1})z_{1,(i)}^{k} = 0 \text{ in } \Omega_{1}, \\
z_{1,(i)}^{k}(0) = 0, \\
\dot{z}_{1,(i)}^{k}(\alpha) = f_{\alpha,(i)}^{k-1},
\end{cases}
\begin{cases}
\ddot{z}_{2,(i)}^{k} - (d_{i}^{2} + \nu^{-1})z_{2,(i)}^{k} = 0 \text{ in } \Omega_{2}, \\
z_{2,(i)}^{k}(\alpha) = z_{1,(i)}^{k}(\alpha), \\
\dot{z}_{2,(i)}^{k}(T) + d_{i}z_{2,(i)}^{k}(T) = -\gamma\nu^{-1}z_{2,(i)}^{k}(T),
\end{cases}$$

where we still update the transmission condition by (3.24). Note that both algo-385 386 rithms (3.23) and (3.25) are of ND type.

Using the solutions (3.5) and the transmission condition in (3.24), we obtain 387

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$$A_i^k = \frac{f_{\alpha,(i)}^{k-1}}{\sigma_i \cosh(a_i)}, B_i^k = \frac{f_{\alpha,(i)}^{k-1} \tanh(a_i)/\sigma_i}{\sigma_i \cosh(b_i) + \omega_i \sinh(b_i)},$$
 and we therefore get for the update condition (3.24) $f_{\alpha,(i)}^k = (1-\theta)f_{\alpha,(i)}^{k-1} - \theta f_{\alpha,(i)}^{k-1} \tanh(a_i) \frac{\sigma_i \sinh(b_i) + \omega_i \cosh(b_i)}{\sigma_i \cosh(b_i) + \omega_i \sinh(b_i)}.$

389 dition (3.24)
$$f_{\alpha_i(i)}^k = (1 - \theta) f_{\alpha_i(i)}^{k-1} - \theta f_{\alpha_i(i)}^{k-1} \tanh(a_i) \frac{\sigma_i \sinh(b_i) + \omega_i \cosh(b_i)}{\sigma_i \cosh(b_i) + \omega_i \sinh(b_i)}$$

THEOREM 3.18. The algorithm ND_2 (3.23)-(3.24) converges if and only if 390

391 (3.26)
$$\rho_{ND_2} := \max_{d_i \in \lambda(A)} \left| 1 - \theta \left(1 + \tanh(a_i) \frac{\sigma_i \tanh(b_i) + \omega_i}{\sigma_i + \omega_i \tanh(b_i)} \right) \right| < 1.$$

COROLLARY 3.19. The algorithm ND_2 for $\theta = 1$ converges if $\alpha \leq \frac{T}{2}$. 392

Proof. Substituting $\theta = 1$ into (3.26), we have

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394 (3.27)
$$\rho_{\text{ND}_2}|_{\theta=1} = \max_{d_i \in \lambda(A)} \left| \tanh(a_i) \frac{\sigma_i \tanh(b_i) + \omega_i}{\sigma_i + \omega_i \tanh(b_i)} \right|.$$

Since $0 < \tanh(x) < 1, \forall x > 0$, both the numerator and the denominator in (3.27) 395

are positive. In the case where $a_i \leq b_i$ (i.e., $\alpha \leq T - \alpha$), we have $\tanh(a_i) \leq \tanh(b_i)$, 396

and the difference between the numerator and the denominator is $\tanh(a_i)(\omega_i +$ 397

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398
$$\sigma_i \tanh(b_i) - (\sigma_i + \omega_i \tanh(b_i)) = \omega_i (\tanh(a_i) - \tanh(b_i)) + \sigma_i (\tanh(b_i) \tanh(a_i) - 1) < 0$$
, meaning that $0 < \tanh(a_i) \frac{\sigma_i \tanh(b_i) + \omega_i}{\sigma_i + \omega_i \tanh(b_i)} < 1$. This concludes the proof.

As shown in Corollary 3.15, the algorithm DN₂ (3.16)-(3.17) with $\theta = 1$ does not converge for $\alpha \leq \frac{T}{2}$, whereas the algorithm ND₂ (3.23)-(3.24) converges in this case. This reveals a symmetry behavior, since the only difference between these two algorithms is that we exchange the Dirichlet and the Neumann condition in the two subdomains. This symmetry is well-known for classical DN and ND algorithms.

Corollary 3.20. For $\gamma = 0$, the algorithm ND₂ for $\theta = 1$ converges for all 405 initial quesses. 406

Proof. This is shown in Corollary 3.19 for $\alpha \leq \frac{T}{2}$. If $\alpha > \frac{T}{2}$, i.e. $a_i > b_i$, then $\tanh(a_i) > \tanh(b_i)$, and the difference between the numerator and the denominator is $\tanh(a_i)(d_i+\sigma_i\tanh(b_i))-(\sigma_i+d_i\tanh(b_i))=(\tanh(b_i)\tanh(a_i)-1)(\sigma_i-d_i)(\sigma_i-d_i)$ (b_i)) < 0, where we use the fact that $0 < \sigma_i - d_i < \sigma_i - d_i \tanh(a_i - b_i)$. This shows that the algorithm ND₂ for $\theta = 1$ converge for $\alpha > \frac{T}{2}$ in the case $\gamma = 0$.

Notice that the matrix A here can be singular, in contrast to the algorithm DN_1 412 413 in Corollary 3.4 where non-singularity is needed for A. As in the previous section, we can still show the convergence behavior for extreme eigenvalues. If the eigenvalue 414 415 $d_i = 0$, we find

416 (3.28)
$$\rho_{\text{ND}_2}|_{d_i=0} = \left| 1 - \theta \left(1 + \tanh(\sqrt{\nu^{-1}}\alpha) \frac{\tanh(\sqrt{\nu^{-1}}(T-\alpha)) + \gamma\sqrt{\nu^{-1}}}{1 + \gamma\sqrt{\nu^{-1}}\tanh(\sqrt{\nu^{-1}}(T-\alpha))} \right) \right|.$$

The expression (3.28) is very similar to (3.21): when $\gamma = 0$, the convergence fac-417

tor (3.21) becomes $\rho_{\text{DN}_2}|_{d_i=0,\gamma=0} = |1 - \theta(1 + \coth(\sqrt{\nu^{-1}}\alpha) \coth(\sqrt{\nu^{-1}}(T-\alpha)))|$, 418

whereas (3.28) becomes $\rho_{ND_2}|_{d_i=0,\gamma=0} = |1-\theta(1+\tanh(\sqrt{\nu^{-1}}\alpha)\tanh(\sqrt{\nu^{-1}}(T-\alpha)))|$. 419

We find again the symmetry between DN₂ and ND₂. In the case when the eigenvalue 420

goes to infinity, using Remark 3.6, we obtain $\lim_{d_1\to\infty}\rho_{ND_2}=|1-2\theta|$, as for DN₂. 421

By equioscillating the convergence factor again for small and large eigenvalues, we

obtain after some computations the relaxation parameter 423

$$\theta_{ND_2}^* = \frac{2}{3 + \tanh(\sqrt{\nu^{-1}}\alpha) \frac{\tanh(\sqrt{\nu^{-1}}(T-\alpha)) + \gamma\sqrt{\nu^{-1}}}{1 + \gamma\sqrt{\nu^{-1}}\tanh(\sqrt{\nu^{-1}}(T-\alpha))}}.$$

- We thus obtain a similar result as Theorem 3.17. 425
- THEOREM 3.21. If we assume that the eigenvalues of A are anywhere in the inter-426 val $[0,\infty)$, then the optimal relaxation parameter $\theta_{ND_2}^{\star}$ for the algorithm ND_2 (3.23)-427
- (3.24) with $\gamma = 0$ is given by (3.29), and satisfies $\frac{1}{2} < \theta_{ND_2}^{\star} < \frac{2}{3}$. 428
- *Proof.* As for Theorem 3.17, we take the derivative of ρ_{ND_2} with respect to 429

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$$d_i$$
, $\frac{d\rho_{\text{ND}_2}}{dd_i} = \frac{d_i \alpha}{\sigma_i \cosh^2(a_i)} \frac{\sigma_i \tanh(b_i) + \omega_i}{\sigma_i + \omega_i \tanh(b_i)} + \frac{\nu^{-1} \tanh(a_i)}{\sigma_i} \frac{\beta_i (1 - \tanh^2(b_i)) - \frac{d_i (T - \alpha)}{\cosh^2(b_i)} (\gamma^2 \nu^{-1} + 2d_i \gamma - 1)}{(\sigma_i + \omega_i \tanh(b_i))^2}$, with σ_i , ω_i and β_i defined in (2.8). For $\gamma = 0$, the derivative is positive and thus ρ_{ND_2}

- 431
- increases with d_i . Therefore $\theta_{ND_2}^*$ is determined by equioscillation. Inserting $\gamma = 0$ 432
- into (3.29), the denominator becomes $3 + \tanh(\sqrt{\nu^{-1}}\alpha) \tanh(\sqrt{\nu^{-1}}(T-\alpha)) < 4$.
- As for DN₂ however, the monotonicity of the convergence factor ρ_{ND_2} is not guar-434 anteed for $\gamma > 0$, and the optimal relaxation parameter $\theta_{ND_2}^{\star}$ may differ from (3.29). 435
- 3.3. Category III. We finally study algorithms in Category III which run only 436 on the state $\mu_{(i)}$ to solve the problem (2.4), and use DN and ND techniques. 437
- **3.3.1. Dirichlet-Neumann algorithm (DN** $_3$). As shown in Table 1, we apply 438 439 the Dirichlet condition in Ω_1 and the Neumann condition in Ω_2 , both to the state $\mu_{(i)}$. For iteration index $k = 1, 2, \dots$, the algorithm DN₃ solves 440

$$\begin{cases} \begin{pmatrix} \dot{z}_{1,(i)}^{k} \\ \dot{\mu}_{1,(i)}^{k} \end{pmatrix} + \begin{pmatrix} d_{i} & -\nu^{-1} \\ -1 & -d_{i} \end{pmatrix} \begin{pmatrix} z_{1,(i)}^{k} \\ \mu_{1,(i)}^{k} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \text{ in } \Omega_{1}, \\ z_{1,(i)}^{k}(0) = 0, \\ \mu_{1,(i)}^{k}(\alpha) = f_{\alpha,(i)}^{k-1}, \\ \begin{pmatrix} \dot{z}_{2,(i)}^{k} \\ \dot{\mu}_{2,(i)}^{k} \end{pmatrix} + \begin{pmatrix} d_{i} & -\nu^{-1} \\ -1 & -d_{i} \end{pmatrix} \begin{pmatrix} z_{2,(i)}^{k} \\ \mu_{2,(i)}^{k} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \text{ in } \Omega_{2}, \\ \dot{\mu}_{2,(i)}^{k}(\alpha) = \dot{\mu}_{1,(i)}^{k}(\alpha), \\ \mu_{2,(i)}^{k}(T) + \gamma z_{2,(i)}^{k}(T) = 0, \end{cases}$$

and we update the transmission condition by 442

443 (3.31)
$$f_{\alpha,(i)}^k := (1 - \theta) f_{\alpha,(i)}^{k-1} + \theta \mu_{2,(i)}^k(\alpha), \theta \in (0,1).$$

- The forward-backward structure is now less present in Ω_2 , where we would expect 444
- to have an initial condition for $z_{2,(i)}$ instead of $\mu_{2,(i)}$. By using the identity of $\mu_{(i)}$ 445
- in (2.5), we can interpret the Neumann condition $\dot{\mu}_{2,(i)}^k(\alpha) = \dot{\mu}_{1,(i)}^k(\alpha)$ as $d_i \dot{z}_{2,(i)}^k(\alpha) +$ 446
- $\sigma_i^2 z_{2,(i)}^k(\alpha) = d_i \dot{z}_{1,(i)}^k(\alpha) + \sigma_i^2 z_{1,(i)}^k(\alpha)$, a Robin type condition on $z_{2,(i)}$. Therefore, the 447
- algorithm DN₃ can also be interpreted as a DR algorithm. 448
- For the convergence analysis, it is natural to choose the interpretation in $\mu_{(i)}$, i.e., 449 using (2.7), which gives 450

$$\begin{cases}
\ddot{\mu}_{1,(i)}^{k} - \sigma_{i}^{2} \mu_{1,(i)}^{k} = 0 \text{ in } \Omega_{1}, \\
\dot{\mu}_{(i)}(0) - d_{i} \mu_{(i)}(0) = 0, \\
\mu_{1,(i)}^{k}(\alpha) = f_{\alpha,(i)}^{k-1},
\end{cases}
\begin{cases}
\ddot{\mu}_{2,(i)}^{k} - \sigma_{i}^{2} \mu_{2,(i)}^{k} = 0 \text{ in } \Omega_{2}, \\
\dot{\mu}_{2,(i)}^{k}(\alpha) = \dot{\mu}_{1,(i)}^{k}(\alpha), \\
\gamma \dot{\mu}_{(i)}(T) + \beta_{i} \mu_{(i)}(T) = 0,
\end{cases}$$

where we still update the transmission condition through (3.31). We observe that 452 both (3.30) and (3.32) are DN type algorithms. Proceeding as before, we obtain: 453

Theorem 3.22. The algorithm DN_3 (3.30)-(3.31) converges if and only if 454

$$(3.33) \qquad \rho_{DN_3} := \max_{d_i \in \lambda(A)} \left| 1 - \theta \left(1 + \frac{\sigma_i + d_i \coth(a_i)}{\sigma_i \coth(a_i) + d_i} \frac{\gamma \sigma_i \coth(b_i) + \beta_i}{\gamma \sigma_i + \beta_i \coth(b_i)} \right) \right| < 1.$$

To get more insight, we choose $\theta = 1$ in (3.33), and find 456

$$\rho_{\mathrm{DN}_3}|_{\theta=1} = \max_{d_i \in \lambda(A)} \left| \frac{\sigma_i + d_i \coth(a_i)}{\sigma_i \coth(a_i) + d_i} \frac{\gamma \sigma_i \coth(b_i) + \beta_i}{\gamma \sigma_i + \beta_i \coth(b_i)} \right|.$$

It is less clear whether $\gamma \sigma_i + \beta_i \coth(b_i)$ is positive, since, using the definition of β_i 458

and
$$\sigma_i$$
 from (2.8), we have $\gamma \sigma_i + \beta_i \coth(b_i) = \gamma(\sqrt{d_i^2 + \nu^{-1}} - d_i \coth(\sqrt{d_i^2 + \nu^{-1}}))$

- (α)) + coth $(\sqrt{d_i^2 + \nu^{-1}}(T \alpha))$, and depending on the values of ν, γ and α , this could 460
- be negative. However, we can simplify (3.34) by setting $\gamma = 0$, and obtain: 461
- COROLLARY 3.23. If $\gamma = 0$, then the algorithm DN₃ with $\theta = 1$ converges for all 462 initial guesses. 463
- 464 *Proof.* Substituting $\theta = 1$ into (3.34), we have

$$\rho_{\mathrm{DN}_3}|_{\theta=1} = \max_{d_i \in \lambda(A)} \left| \frac{\sigma_i \tanh(a_i) + d_i}{\sigma_i + d_i \tanh(a_i)} \tanh(b_i) \right|.$$

- Both the numerator and the denominator are positive. Using $0 < \tanh(x) < 1$, 466
- $\forall x > 0$, we get $(d_i + \sigma_i \tanh(a_i)) (\sigma_i + d_i \tanh(a_i)) = (d_i \sigma_i)(1 \tanh(a_i)) < 0$, meaning that $0 < \tanh(b_i) \frac{\sigma_i \tanh(a_i) + d_i}{\sigma_i + d_i \tanh(a_i)} < 1$, which concludes the proof. 467
- 468
- For $\gamma = 0$, the algorithm DN₃ (3.30)-(3.31) converges for $\theta = 1$ as well as the 469
- algorithm ND₂ (3.23)-(3.24), since their convergence factors are very similar. For ex-470
- treme eigenvalues, inserting $d_i = 0$ into (3.33), we find the identical formula as (3.28), 471
- and when the eigenvalue goes to infinity, we also obtain $\lim_{d_1\to\infty} \rho_{DN_3} = |1-2\theta|$. By 472
- equioscillating the convergence factor between small and large eigenvalues, we obtain 473
- thus the same relaxation parameter as (3.29), which leads to: 474
- THEOREM 3.24. If we assume the eigenvalues of A can be anywhere in the interval 475
- $[0,\infty)$, then the optimal relaxation parameter $\theta_{DN_3}^{\star}$ for the algorithm DN_3 (3.30)-(3.31) 476
- with $\gamma = 0$ is identical to $\theta_{ND_2}^{\star}$. 477
- *Proof.* For $\gamma = 0$, the convergence factors (3.27) and (3.35) become the same 478
- when exchanging a_i and b_i , and the result thus follows as for Theorem 3.21. 479
- **3.3.2.** Neumann-Dirichlet algorithm (ND_3) . We now exchange the Dirichlet 480 let and Neumann conditions on the two subdomains, and obtain

$$\begin{cases} \left(\dot{z}_{1,(i)}^{k}\right) + \left(d_{i} - \nu^{-1}\right) \begin{pmatrix} z_{1,(i)}^{k} \\ \mu_{1,(i)}^{k} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \text{ in } \Omega_{1}, \\ z_{1,(i)}^{k}(0) = 0, \\ \dot{\mu}_{1,(i)}^{k}(\alpha) = f_{\alpha,(i)}^{k-1}, \\ \left(\dot{z}_{2,(i)}^{k} \\ \dot{\mu}_{2,(i)}^{k} \end{pmatrix} + \begin{pmatrix} d_{i} - \nu^{-1} \\ -1 - d_{i} \end{pmatrix} \begin{pmatrix} z_{2,(i)}^{k} \\ \mu_{2,(i)}^{k} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \text{ in } \Omega_{2}, \\ \mu_{2,(i)}^{k}(\alpha) = \mu_{1,(i)}^{k}(\alpha), \\ \mu_{2,(i)}^{k}(T) + \gamma z_{2,(i)}^{k}(T) = 0, \end{cases}$$

where the transmission condition is updated by 483

484 (3.37)
$$f_{\alpha,(i)}^{k} := (1 - \theta) f_{\alpha,(i)}^{k-1} + \theta \dot{\mu}_{2,(i)}^{k}(\alpha), \theta \in (0,1).$$

As for DN₃, we need to use the identity (2.5) and interpret $\mu_{2,(i)}^k(\alpha) = \mu_{1,(i)}^k(\alpha)$ as 485

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$$\dot{z}_{2,(i)}^k(\alpha) + d_i z_{2,(i)}^k(\alpha) = \dot{z}_{1,(i)}^k(\alpha) + d_i z_{1,(i)}^k(\alpha)$$
 to reveal the forward-backward structure
487 with a NR type algorithm. Using formulation (2.7), we get

$$\begin{cases}
\ddot{\mu}_{1,(i)}^{k} - \sigma_{i}^{2} \mu_{1,(i)}^{k} = 0 \text{ in } \Omega_{1}, \\
\dot{\mu}_{(i)}(0) - d_{i} \mu_{(i)}(0) = 0, \\
\dot{\mu}_{1,(i)}^{k}(\alpha) = f_{\alpha,(i)}^{k-1},
\end{cases}
\begin{cases}
\ddot{\mu}_{2,(i)}^{k} - \sigma_{i}^{2} \mu_{2,(i)}^{k} = 0 \text{ in } \Omega_{2}, \\
\mu_{2,(i)}^{k}(\alpha) = \mu_{1,(i)}^{k}(\alpha), \\
\gamma \dot{\mu}_{(i)}(T) + \beta_{i} \mu_{(i)}(T) = 0.
\end{cases}$$

THEOREM 3.25. The algorithm ND₃ (3.36)-(3.37) converges if and only if 489

490 (3.39)
$$\rho_{ND_3} := \max_{d_i \in \lambda(A)} \left| 1 - \theta \left(1 + \frac{\sigma_i + d_i \tanh(a_i)}{\sigma_i \tanh(a_i) + d_i} \frac{\gamma \sigma_i \tanh(b_i) + \beta_i}{\gamma \sigma_i + \beta_i \tanh(b_i)} \right) \right| < 1.$$

As in the previous section, we choose $\theta = 1$ in (3.39), and find 491

492 (3.40)
$$\rho_{\text{ND}_3}|_{\theta=1} = \max_{d_i \in \lambda(A)} \left| \frac{\sigma_i + d_i \tanh(a_i)}{\sigma_i \tanh(a_i) + d_i} \frac{\gamma \sigma_i \tanh(b_i) + \beta_i}{\gamma \sigma_i + \beta_i \tanh(b_i)} \right|.$$

- Again, using the definition of β_i and σ_i from (2.8), we have $\gamma \sigma_i \tanh(b_i) + \beta_i =$ 493
- $\gamma(\sqrt{d_i^2+\nu^{-1}}\tanh(\sqrt{d_i^2+\nu^{-1}}(T-\alpha))-d_i)+1$, and depending on the values of ν,γ 494
- and α , this could be negative. However, we can simplify (3.40) by taking $\gamma = 0$, and
- then obtain the following result. 496

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- COROLLARY 3.26. If $\gamma = 0$, then the algorithm ND_3 with $\theta = 1$ does not converge. 497
- *Proof.* Inserting $\gamma = 0$ into (3.40), we get 498

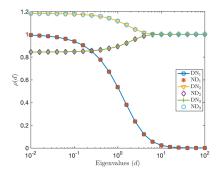
499 (3.41)
$$\rho_{\mathrm{DN}_3}|_{\theta=1} = \max_{d_i \in \lambda(A)} \left| \frac{\sigma_i \coth(a_i) + d_i}{\sigma_i + d_i \coth(a_i)} \coth(b_i) \right|.$$

Both the numerator and the denominator are positive. Using $\coth(x) \ge 1, \forall x > 0$, 500 we find $(d_i + \sigma_i \coth(a_i)) - (\sigma_i + d_i \coth(a_i)) = (\sigma_i - d_i)(\coth(a_i) - 1) > 0$, implying 501 that $\frac{\sigma_i \coth(a_i) + d_i}{\sigma_i + d_i \coth(a_i)} \coth(b_i) > 1$, which concludes the proof. 502

Comparing Corollaries 3.23 and 3.26, we find again a symmetry if $\gamma = 0$, as for Corollaries 3.15 and 3.19, and with $\theta = 1$, ND₃ diverges like DN₂ when $\gamma = 0$. In fact, in this case, the convergence factor of ND₃ (3.41) is very similar to the convergence factor of DN_2 (3.20). Due to this divergence, we cannot provide a general estimate of the convergence factor. We can however still study the convergence behavior for extreme eigenvalues. Inserting $d_i = 0$ into (3.39), we find also (3.21), and thus for small eigenvalues ND₃ behaves like DN₂, like we observed for ND₂ and DN₃ earlier. When the eigenvalue goes to infinity, we also obtain $\lim_{d_i \to \infty} \rho_{ND_3} = |1 - 2\theta|$. Hence all the four algorithms DN₂, ND₂, DN₃ and ND₃ have the same limit for large eigenvalues. By equioscillation, we then obtain the same relaxation parameter as (3.22). This leads to a similar result as Theorem 3.17.

Theorem 3.27. If we assume that the eigenvalues of A are anywhere in the inter-514 val $[0,\infty)$, then the optimal relaxation parameter $\theta_{ND_3}^{\star}$ for the algorithm ND_3 (3.36)-515 (3.37) with $\gamma = 0$ is identical to $\theta_{DN_2}^{\star}$.

Proof. In the case $\gamma = 0$, the convergence factors (3.20) and (3.41) are the same 517 when exchanging a_i and b_i , and thus the proof follows as for Theorem 3.17. 518



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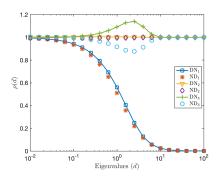


Fig. 2. Convergence factor with $\theta = 1$ for a symmetric decomposition of the six new algorithms as function of the eigenvalues $d \in [10^{-2}, 10^2]$. Left: $\gamma = 0$. Right: $\gamma = 10$.

4. Numerical experiments. We illustrate now our six new time domain decomposition algorithms with numerical experiments. We divide the time domain $\Omega = (0,1)$ into two non-overlapping subdomains with interface α , and fix the regularization parameter $\nu = 0.1$. We will investigate the performance by plotting the convergence factor as function of the eigenvalues $d \in [10^{-2}, 10^2]$.

4.1. Convergence factor with $\theta = 1$ for a symmetric decomposition. We show in Figure 2 the convergence factors for all six algorithms for a symmetric decomposition, $\alpha = \frac{1}{2}$, with $\theta = 1$, on the left without final target state (i.e., $\gamma = 0$), and on the right with a final target state for $\gamma = 10$. Without final target state, the convergence factor of DN₁ and ND₁ coincide, as one can see also by substituting $\gamma = 0$ and $a_i = b_i$ into (3.7) and (3.14). The same also holds for the pairs DN₂ and ND_3 , and DN_3 and ND_2 . We also see the symmetry between DN_2 and ND_2 , as well as DN₃ and ND₃. This changes when a final target state with $\gamma = 10$ is present: while the convergence behavior remains similar for DN_1 and ND_1 , the symmetry between DN₂ and ND₂¹ and DN₃ and ND₃ remains. Furthermore, DN₃ converges with no final target but diverges with $\gamma = 10$, and vice versa for ND₃. In terms of the convergence speed, DN₁ and ND₁ are much better than the other four algorithms for high frequencies in both cases, and ND₁ is slightly better overall than DN₁ when $\gamma = 10$. The good high frequency behavior follows from our analysis: it depends for all 6 algorithms only on θ . In the case $\theta = 1$ here, the limit is $|1 - \theta| = 0$ for DN₁ and ND_1 , and $|1-2\theta|=1$ for DN_2 , DN_3 , ND_2 and ND_3 . For the zero frequency, d=0, the convergence factor for DN₁ and ND₁ equals 1 for all γ , but for DN₂, DN₃, ND_2 and ND_3 this depends on γ . Inserting $\theta = 1$ into (3.21) and (3.28), we obtain for DN₂ and ND₃ the convergence factor $\coth(\sqrt{\nu^{-1}}\alpha)\frac{\sqrt{\nu^{-1}}\coth(\sqrt{\nu^{-1}}\alpha)+\nu^{-1}\gamma}{\sqrt{\nu^{-1}}+\nu^{-1}\gamma\coth(\sqrt{\nu^{-1}}\alpha)}$, and for ND₂ and DN₃ $\tanh(\sqrt{\nu^{-1}}\alpha)\frac{\sqrt{\nu^{-1}}\tanh(\sqrt{\nu^{-1}}\alpha)+\nu^{-1}\gamma}{\sqrt{\nu^{-1}}+\nu^{-1}\gamma\tanh(\sqrt{\nu^{-1}}\alpha)}$. For $\gamma=0$, the two convergence factors are approximately 1.185 for DN₂ and ND₃, 0.844 for ND₂ and DN₃, and for $\gamma = 10$, we get 1.005 for DN₂ and ND₃, and 0.995 ND₂ and DN₃.

4.2. Convergence factor with $\theta = 1$ for an asymmetric decomposition. For $\theta = 1$, we show on the left in Figure 3 the convergence factors with interface at $\alpha = 0.3$ and no final target state (i.e., $\gamma = 0$), and on the right $\alpha = 0.7$ with a final

 $^{^{1}}$ This is a bit hard to see on the right in Figure 2, but zooming in confirms that the convergence factor of DN_{2} is above 1, and below 1 for ND_{2} .

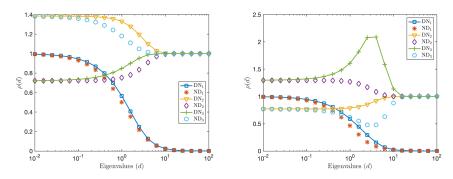


Fig. 3. Convergence factor with $\theta=1$ for an asymmetric decomposition of all six new algorithms as function of the eigenvalues $d \in [10^{-2}, 10^2]$. Left: $\gamma=0$ and $\alpha=0.3$. Right: $\gamma=10$ and $\alpha=0.7$.

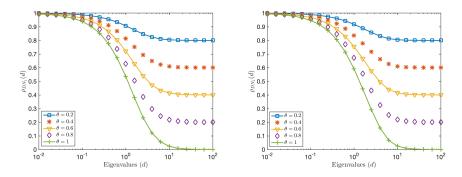


Fig. 4. Convergence factor with different relaxation parameters of DN_1 as function of the eigenvalues $d \in [10^{-2}, 10^2]$. Left: $\gamma = 0$ and $\alpha = 0.5$. Right: $\gamma = 10$ and $\alpha = 0.7$.

target state $\gamma=10$. For DN₁ and ND₁, the convergence factor is similar in both cases, ND₁ being slightly better, and convergence is also similar to the symmetric case. This is because the convergence factor of the two algorithms for small and large eigenvalues is independent of the values of α, ν and γ . Their high frequency behavior is also much better compared to the other four algorithms in the two cases. For the other four algorithms, we see again the symmetry between DN₂ and ND₂, and DN₃ and ND₃. In general, DN₂ and ND₃ behave similarly, and also ND₂ and DN₃, but the influence of γ is more significant for DN₃ and ND₃ than DN₂ and ND₂. However their convergence factors all go to 1 for large eigenvalues, as for the symmetric decomposition. For the zero frequency, using the expressions (3.21) and (3.28) with $\theta=1$, we obtain approximately 1.386 for DN₂ and ND₃, and 0.722 for ND₂ and DN₃ in the case $\gamma=0$, $\alpha=0.3$. For $\gamma=10$, $\alpha=0.7$, we get 0.771 for DN₂ and ND₃, and 1.296 for ND₂ and DN₃.

4.3. Convergence factor for Category I with different θ . Since DN_1 and ND_1 performed quite similarly, and much better than the others, we now investigate the dependence of DN_1 on θ in more detail. On the left in Figure 4 we show the convergence factor of DN_1 without final target state and a symmetric decomposition, and on the right with a final target state $\gamma = 10$ and an asymmetric decomposition. The convergence is very similar for these two settings, DN_1 is robust, and $\theta = 1$ gives the best performance.

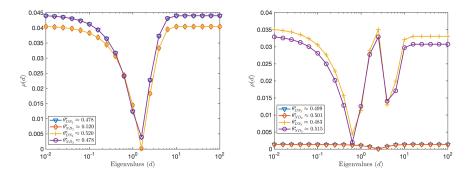


Fig. 5. Convergence factor with θ^* for a symmetric decomposition as function of the eigenvalues $d \in [10^{-2}, 10^2]$. Left: $\gamma = 0$. Right: $\gamma = 10$.

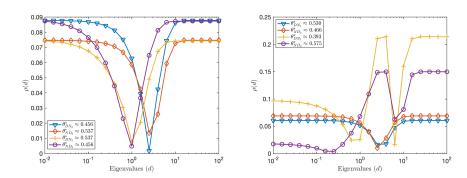


Fig. 6. Convergence factor with θ^* for an asymmetric decomposition as function of the eigenvalues $d \in [10^{-2}, 10^2]$. Left: $\gamma = 0$ and $\alpha = 0.3$. Right: $\gamma = 10$ and $\alpha = 0.7$.

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4.4. Convergence factor with optimal θ for a symmetric decomposition. Since the algorithms in Categories II and III are strongly related, we compare them now in Figure 5 for a symmetric decomposition using their optimal relaxation parameter θ^* , obtained numerically. On the left without final state, DN₂ and ND₃, and also ND₂ and DN₃, have the same convergence factor, and the optimal relaxation parameter satisfies $\theta_{\mathrm{DN}_2}^{\star} = \theta_{\mathrm{ND}_3}^{\star}$ and $\theta_{\mathrm{ND}_2}^{\star} = \theta_{\mathrm{DN}_3}^{\star}$ as proved in Theorem 3.24 and Theorem 3.27. These correspond to the value found using (3.22) and (3.29). In terms of the convergence speed, ND₂ and DN₃ are slightly better than DN₂ and ND₃. However, these similarities disappear when we add a final target state $\gamma = 10$. On the right in Figure 5, we see that now the convergence behavior of DN₂ and ND₂ is similar, and also DN₃ and ND₃ are rather similar, and DN₂ and ND₂ converge much faster compared to the others. We also see equioscillation between small and large eigenvalues. The theoretical results in (3.22) as well as in (3.29) still determine the optimal relaxation parameter $\theta_{DN_2}^{\star}$ and $\theta_{ND_2}^{\star}$ for DN₂ and ND₂, but not for DN₃ and ND₃, where we observe an equioscillation between small eigenvalues with some eigenvalues in the interval [1, 10]. Also ND₃ is slightly better than DN₃.

4.5. Convergence factor with optimal θ for an asymmetric decomposition. We show in Figure 6 the convergence factor with the optimal relaxation parameter θ^* for the four algorithms in Categories II and III for an asymmetric decomposition. On the left with $\alpha = 0.3$ and no target state $\gamma = 0$ the convergence factors of the four

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algorithms are similar. This is consistent with the monotonicity we proved without 589 final state. The optimal relaxation parameters satisfy $\theta_{\mathrm{DN}_2}^{\star} = \theta_{\mathrm{ND}_3}^{\star}$ and $\theta_{\mathrm{ND}_2}^{\star} = \theta_{\mathrm{DN}_3}^{\star}$, and we can use (3.22) and (3.29) to determine their values. Similar to the symmetric decomposition, ND₂ and DN₃ are slightly better than the others. However, these properties disappear again on the right in Figure 6 when there is a final state $\gamma = 10$. 594 While DN₂ and ND₂ still equioscillate between the small and large eigenvalues, and the optimal relaxation parameter can be determined using (3.22) and (3.29), for DN₃ and ND₃ the equioscillation is between large eigenvalues and some eigenvalues in the 596 interval [1, 10]. Hence, the optimal relaxation parameters for the algorithms DN₃ and 597 ND₃ are different from DN₂ and ND₂. Also DN₂ and ND₂ converge much faster than 598 the other two, and DN_2 is slightly faster than ND_2 . 599

5. Conclusion. We introduced and analyzed six new time domain decomposition methods based on Dirichlet-Neumann and Neumann-Dirichlet techniques for parabolic optimal control problems. Our analysis shows that while at first sight it might be natural to preserve the forward-backward structure in the time subdomains as well, there are better choices that lead to substantially faster algorithms. We find that the algorithms in Categories II and III with optimized relaxation parameter are much faster than the algorithms in Category I, and they can still be identified to be of forward-backward structure using changes of variables. We also found many interesting mathematical connections between these algorithms. Algorithms in Category I are natural smoothers, while algorithms in Categories II and III with optimized relaxation parameter are highly efficient solvers.

Our study was restricted to the two subdomain case, but the algorithms can all naturally be written for many subdomains, and then one can also run them in parallel. They can also be used for more general parabolic constraints than the heat equation. Extensive numerical results will appear elsewhere.

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Appendix A. Convergence analysis using $\mu_{(i)}$.

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We can also use formulation (2.7) to analyze the convergence behavior of the algorithm DN_1 (3.1)-(3.2), we then need to study

$$\begin{cases}
\ddot{\mu}_{1,(i)}^{k} - \sigma_{i}^{2} \mu_{1,(i)}^{k} = 0 \text{ in } \Omega_{1}, \\
\dot{\mu}_{(i)}(0) - d_{i}\mu_{(i)}(0) = 0, \\
\mu_{1,(i)}^{k}(\alpha) = f_{\alpha,(i)}^{k-1},
\end{cases}
\begin{cases}
\ddot{\mu}_{2,(i)}^{k} - \sigma_{i}^{2} \mu_{2,(i)}^{k} = 0 \text{ in } \Omega_{2}, \\
\ddot{\mu}_{2,(i)}^{k}(\alpha) - d_{i}\dot{\mu}_{2,(i)}^{k}(\alpha) = \ddot{\mu}_{1,(i)}^{k}(\alpha) - d_{i}\dot{\mu}_{1,(i)}^{k}(\alpha), \\
\gamma\dot{\mu}_{(i)}(T) + \beta_{i}\mu_{(i)}(T) = 0,
\end{cases}$$

706 with the update of the transmission condition

707 (A.2)
$$f_{\alpha,(i)}^{k} = (1 - \theta) f_{\alpha,(i)}^{k-1} + \theta \mu_{2,(i)}^{k}(\alpha) \quad \theta \in (0, 1).$$

This is a DR type algorithm applied to solve (2.7). Using (3.12), we determine the two coefficients A_i^k and B_i^k from the transmission condition from (A.1). Using then relation (A.2), we find

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$$f_{\alpha,(i)}^{k} = (1-\theta)f_{\alpha,(i)}^{k-1} + \theta\nu^{-1}f_{\alpha,(i)}^{k-1} \frac{\gamma\sigma_{i} + \beta_{i}\tanh(b_{i})}{\left(\sigma_{i} + d_{i}\tanh(a_{i})\right)\left(\omega_{i} + \sigma_{i}\tanh(b_{i})\right)},$$

712 which is exactly the same convergence factor as (3.6).

Appendix B. 1D Advection-diffusion problems. We can also consider the operator $\partial_x - \kappa \partial_{xx}$, and use a finite difference scheme to discretize it, for instance, an upwind discretization for the advection part ∂_x and the standard centred discretization for the diffusion part ∂_{xx} . With mesh size h, the eigenfunctions in this case are $e^{in\pi jh}$ with eigenvalues $d_n := 2(\frac{1}{h} + \kappa \frac{2}{h^2}) \sin^2(\frac{n\pi h}{2}) + i\frac{1}{h} \sin(n\pi h)$. As presented in Section 4, we can then check the convergence behavior of the proposed algorithms for advection-diffusion problems. As an example, we keep the same setting as for Figure 5, but now use the eigenvalues from above. We show in Figure 7 the convergence factor with respect to the eigenvalues for diffusion coefficient $\kappa = 10^{-1}$ and $\kappa = 10^{-2}$. Comparing with the pure diffusion case in Figure 5, we see that adding an advection term leads to slower convergence, while the order from best to worst algorithm is maintained as for pure diffusion, both for $\gamma = 0$ (left) and $\gamma = 10$ (right). For $\gamma = 10$, the slower algorithm variants even tend to stagnate as the problem becomes advection dominant, but the fast algorithms remain fast in that case, see Figure 5 (right). We also see that the optimized relaxation parameters depend on the presence of advection.

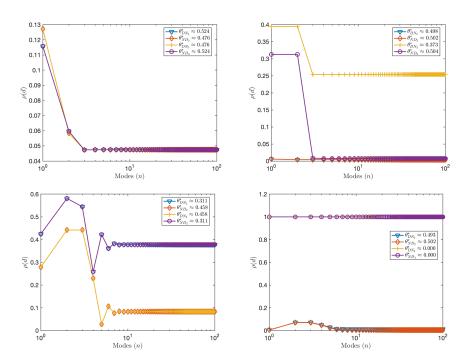


Fig. 7. Convergence factor with θ^* for a symmetric decomposition as function of the eigenvalues $d_n = 2(\frac{1}{h} + \kappa \frac{2}{h^2})\sin^2(\frac{n\pi h}{2}) + i\frac{1}{h}\sin(n\pi h), \ n \in [10^0, 10^2].$ Top: $\kappa = 10^{-1}$. Bottom: $\kappa = 10^{-2}$. Left: $\gamma = 0$. Right: $\gamma = 10$.