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A HOMOGRAPHIC BEST APPROXIMATION PROBLEM WITH APPLICATION TO OPTIMIZED SCHWARZ WAVEFORM RELAXATION

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Abstract. We present and study a homographic best approximation problem, which arises in the analysis of waveform relaxation algorithms with optimized transmission conditions. Its solution characterizes in each class of transmission conditions the one with the best performance of the associated waveform relaxation algorithm. We present the particular class of first order transmission conditions in detail and show that the new waveform relaxation algorithms are well posed and converge much faster than the classical one: the number of iterations to reach a certain accuracy can be orders of magnitudes smaller. We illustrate our analysis with numerical experiments.

1. Introduction

Over the last decade, a new domain decomposition method for evolution problems has been developed, the so-called Schwarz waveform relaxation method; see [10, 21, 23, 22] for linear problems, and [11, 20, 24] for nonlinear ones. The new method is well suited for solving evolution problems in parallel in space-time, and it permits not only local adaptation in space, but also in time. A significant drawback of this new method is its slow convergence on long time intervals. This problem can however be remedied by more effective transmission conditions; see [17, 8, 18, 13, 14, 31]. These transmission conditions are of differential type in both time and space, and depend on coefficients which are determined by optimization of the convergence factor. The associated best approximation problem has been studied for the optimized Schwarz waveform relaxation algorithm with Robin transmission conditions applied to the one-dimensional advection-diffusion equation in [15]. In higher dimensions, and for higher order transmission conditions, only numerical procedures have been used so far to solve the associated best approximation problem; see [31, 8]. Here we study this best approximation problem in a more general setting: we search for a given function $f : \mathbb{C} \to \mathbb{C}$ the polynomial $s_n^*(z)$ of degree less than or equal to n, which minimizes the quantity

$$\sup_{z\in K} \left| \frac{s(z) - f(z)}{s(z) + f(z)} e^{-lf(z)} \right| \tag{1.1}$$

over all polynomials s of degree less than or equal to n. Here, K is a closed set in $\mathbb{C}$, and l is a nonnegative real parameter.

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The classical best approximation problem is the following: given a real-valued continuous function on a compact interval and a class of functions defined on the same interval, find an element in the class which realizes the distance of the function to the class. If the class is the linear space of polynomials of degree less than or equal to n, and the distance is measured in the L^∞ norm, then the approximation problem is called a Chebyshev best approximation problem. This problem was studied in depth by Chebyshev and De la Vallée Poussin [32]. Its solution is characterized by an equioscillation property, and can be computed using the Remes algorithm [34, 33]. Later extensions concern rational approximations [5], and functions of a complex variable [38]. In the latter problem, Rivlin and Shapiro obtained equioscillation properties, from which they deduced uniqueness; see [35]. In all cases existence is a matter of compactness. Problem (1.1) generalizes the complex best approximation problem by polynomials in two directions: first the difference $f - s$ is replaced by a homographic function in f and s, and second there can be an exponential weight which involves the function f itself.

2. A general best approximation result

Let K be a closed set in $\mathbb{C}$, containing at least $n+2$ points. Let $f : K \to \mathbb{C}$ be a continuous function, such that for every z in K, $\Re f(z) > 0$. We denote by $\mathbf{P}_n$ the complex vector space of polynomials of degree less than or equal to n. We define, for l nonnegative real number,

$$\delta_n(l) = \inf_{s\in\mathbf{P}_n} \sup_{z\in K} \left| \frac{s(z)-f(z)}{s(z)+f(z)} e^{-lf(z)} \right|, \tag{2.1}$$

and search for s_n^* in $\mathbf{P}_n$ such that

$$\sup_{z\in K} \left| \frac{s_n^*(z)-f(z)}{s_n^*(z)+f(z)} e^{-lf(z)} \right| = \delta_n(l). \tag{2.2}$$

2.1. **Analysis of the case $l = 0$.** We suppose here K is compact. We denote for simplicity by δ_n the number $\delta_n(0)$. Our analysis of (2.2) has three major steps: we first prove existence of a solution, then show that the solution must satisfy an equioscillation property, and finally, using the equioscillation property, we prove uniqueness of the solution. We define for any z_0 in $\mathbb{C}^* = \mathbb{C}\setminus 0$ and strictly positive δ the sets

$$\begin{gathered} \mathcal{C}(z_0,\delta) = \{z\in\mathbb{C}, \left|\tfrac{z-z_0}{z+z_0}\right| = \delta\},\ \mathcal{D}(z_0,\delta) = \{z\in\mathbb{C}, \left|\tfrac{z-z_0}{z+z_0}\right| < \delta\}, \\ \overline{\mathcal{D}}(z_0,\delta) = \mathcal{C}(z_0,\delta)\cup\mathcal{D}(z_0,\delta). \end{gathered} \tag{2.3}$$

The proof of the following geometrical lemma is straightforward; see [1]:

Lemma 2.1. *For any δ different from 0 and 1, and for any z_0 in $\mathbb{C}^* = \mathbb{C}\setminus 0$, the set $\mathcal{C}(z_0,\delta)$ in (2.3) is a circle with center at $\frac{1+\delta^2}{1-\delta^2}z_0$ and radius $\frac{2\delta}{|1-\delta^2|}|z_0|$. If $\delta < 1$, the set $\mathcal{D}(z_0,\delta)$ is the interior of the circle, and the exterior otherwise. The set $\mathcal{C}(z_0,1)$ is a line orthogonal to the line $(0,z_0)$.*

Theorem 2.2 (Existence)**.** *Suppose $l = 0$ and K compact. For every $n \geq 0$, the number $\delta_n = \delta_n(0)$ is strictly smaller than 1, and there exists at least one solution to problem (2.2).*

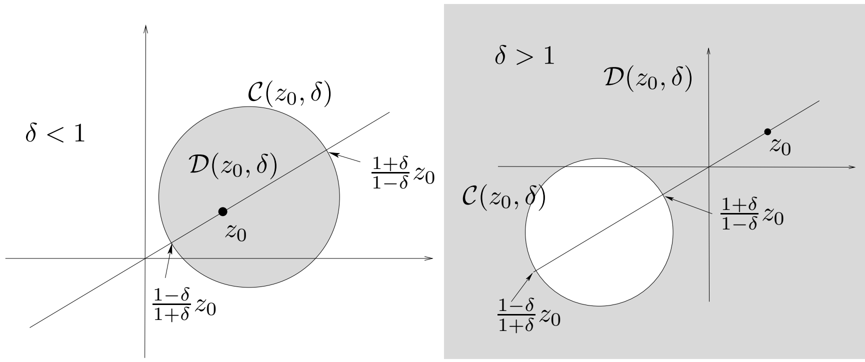

FIGURE 1. Illustration of the geometric Lemma 2.1: definition of $\mathcal{D}(z_0,\delta)$ in grey.

Proof. Since $1 \in \mathbf{P}_n$, we have $\delta_n \leq \left\|\frac{1-f}{1+f}\right\|_\infty$. Now for any z in K, $\Re f(z) > 0$, and therefore $\left|\frac{1-f(z)}{1+f(z)}\right| < 1$. Since K is a compact set, we have $\delta_n < 1$. To prove existence, we take a minimizing sequence $\left(s_n^k\right)_{k\in\mathbb{N}}$ in $\mathbf{P}_n$, such that

$$\lim_{k\to\infty}\left\|\frac{s_n^k - f}{s_n^k + f}\right\|_\infty = \delta_n.$$

There exists a k_0 such that, for $k \geq k_0$, we have $\left\|\frac{s_n^k-f}{s_n^k+f}\right\|_\infty \leq C < 1$ with $C = (1+\delta_n)/2$, and therefore by Lemma 2.1, $\frac{s_n^k}{f}(z)$ lies inside the disk $\overline{\mathcal{D}}(1,C)$, $C<1$, for all z in K. Hence s_n^k is a bounded sequence in the finite dimensional space $\mathbf{P}_n$ and thus there exists a subsequence which converges to some s_n^* in $\mathbf{P}_n$, which attains the infimum. □

We now investigate the equioscillation property of the solutions to (2.2). To do so, we need two further lemmas.

Lemma 2.3. *For a given vector $\boldsymbol{w} = (w_1,\ldots,w_m)$, $m \leq n+1$, such that w_j is in K for every j, let $U_{\boldsymbol{w}}$ be the open set in $\mathbf{P}_n$ of polynomials s such that $s(w_i)+f(w_i) \neq 0$ for all $i = 1,2,\ldots,m$. If $w_i \neq w_j$ for $i \neq j$, the mapping*

$$\mathcal{A}_{\boldsymbol{w}} : U_{\boldsymbol{w}} \to \mathbb{C}^m, \quad s \mapsto \left(\frac{s(w_i)-f(w_i)}{s(w_i)+f(w_i)}\right)_{1\leq i\leq m}$$

is a submersion: for any s in $U_{\boldsymbol{w}}$, the derivative in s, $\mathcal{A}'_{\boldsymbol{w}}(s)$, is onto. Furthermore, the function $(s,w) \mapsto \mathcal{A}'_{\boldsymbol{w}}(s)$ is continuous with respect to s and w.

Proof. The derivative of the mapping $A_{\boldsymbol{w}}$ is given by

$$\mathcal{A}'_{\boldsymbol{w}}(s)\cdot\tilde{s} = \left(\frac{2\tilde{s}(w_i)f(w_i)}{(s(w_i)+f(w_i))^2}\right)_{1\leq i\leq m}, \quad \forall\tilde{s}\in\mathbf{P}_n. \tag{2.4}$$

Now for any $\boldsymbol{z}$ in $\mathbb{C}^m$, there exists a unique polynomial $\tilde{s}$ in $\mathbf{P}_{m-1}$, namely the Lagrange interpolation polynomial, such that

$$\forall i, 1\leq i\leq m,\ \tilde{s}(w_i) = \frac{(s(w_i)+f(w_i))^2}{2f(w_i)}z_i,$$

and since $m-1 \leq n$, $\tilde{s}$ is in $\mathbf{P}_n$ and $\mathcal{A}'_{\boldsymbol{w}}(s)\cdot\tilde{s} = \boldsymbol{z}$. The continuity of $\mathcal{A}'_{\boldsymbol{w}}$ with respect to s and $\boldsymbol{w}$ follows directly from (2.4). $\square$

Lemma 2.4. *Let s_n^* be a solution of* (2.2) *for $l = 0$. Let $\boldsymbol{z} = (z_1,\dots,z_m)$ be a vector of m distinct points in K, $m \leq n+1$. We have*

(1) *s_n^* is in $U_{\boldsymbol{z}}$,*
(2) *let s be such that $\mathcal{A}'_{\boldsymbol{z}}(s_n^*)\ s = -\mathcal{A}_{\boldsymbol{z}}(s_n^*)$. Then for any ϵ, $0<\epsilon<1$, there exist positive $(\epsilon_1,\dots,\epsilon_m)$, and $t_0 \in (0,1)$, such that for any $t \in [\epsilon t_0, t_0]$ and for any z in K with $|z - z_i| < \epsilon_i$ for some i,*

$$\left|\frac{s_n^*(z)+ts(z)-f(z)}{s_n^*(z)+ts(z)+f(z)}\right| \leq (1-\epsilon\frac{t_0}{2})\delta_n.$$

Proof. For (1), s_n^* is in $U_{\boldsymbol{z}}$ since otherwise δ_n would be infinite. For (2), there exist strictly positive numbers $t_0', \epsilon_1', \dots, \epsilon_m'$ such that, for any t in $[0, t_0']$, and any $\boldsymbol{w} = (w_1, w_2, \dots, w_m)$ with $w_j \in K$ and $|w_j - z_j| < \epsilon_j$ for all j, $s_n^* + ts$ is in $U_{\boldsymbol{w}}$. We now define $f_i(t,\boldsymbol{w}) = (\mathcal{A}_{\boldsymbol{w}}(s_n^*+ts))_i$, and we apply to f_i the first order Taylor-Lagrange formula in the first variable, about $t=0$. There exists τ_i in $(0,t)$ such that

$$f_i(t,\boldsymbol{w}) = f_i(0,\boldsymbol{w}) + t\partial_1 f_i(\tau_i,\boldsymbol{w}),$$

and by adding and subtracting $t\partial_1 f_i(0,\boldsymbol{z})$, we obtain

$$f_i(t,\boldsymbol{w}) = f_i(0,\boldsymbol{w}) + t\partial_1 f_i(0,\boldsymbol{z}) + t(\partial_1 f_i(\tau_i,\boldsymbol{w}) - \partial_1 f_i(0,\boldsymbol{z})).$$

Now using that s satisfies the equation $\mathcal{A}'_{\boldsymbol{z}}(s_n^*)s = -\mathcal{A}_{\boldsymbol{z}}(s_n^*)$, which reads componentwise $\partial_1 f_i(0,\boldsymbol{z}) = -f_i(0,\boldsymbol{z})$, we get

$$\begin{aligned} f_i(t,\boldsymbol{w}) &= f_i(0,\boldsymbol{w}) - tf_i(0,\boldsymbol{z}) + t(\partial_1 f_i(\tau_i,\boldsymbol{w}) - \partial_1 f_i(0,\boldsymbol{z})) \\ &= (1-t)f_i(0,\boldsymbol{w}) + t(f_i(0,\boldsymbol{w}) - f_i(0,\boldsymbol{z})) + t(\partial_1 f_i(\tau_i,\boldsymbol{w}) - \partial_1 f_i(0,\boldsymbol{z})). \end{aligned}$$

Since the functions f_i and $\partial_1 f_i$ are continuous in a neighbourhood of $(0,\boldsymbol{z})$, we obtain

$$f_i(t,\boldsymbol{w}) = (1-t)f_i(0,\boldsymbol{w}) + t\eta_i(\boldsymbol{w},\boldsymbol{w}-\boldsymbol{z}),$$

with some function $\eta_i(\boldsymbol{w},\boldsymbol{w}-\boldsymbol{z})$ continuous in $\boldsymbol{w}$, which tends to zero with $\boldsymbol{w}-\boldsymbol{z}$. Thus, for any positive ϵ, there exist positive $\epsilon_1,\dots,\epsilon_m$, and $0<t_0<1$, such that for any t in $[0,t_0]$ and any $\boldsymbol{w} = (w_1,\dots,w_m)$ with $|w_i - z_i| < \epsilon_i$ for all i,

$$\left|\frac{s_n^*(w_i)+ts(w_i)-f(w_i)}{s_n^*(w_i)+ts(w_i)+f(w_i)}\right| \leq (1-t)\delta_n + \epsilon\delta_n\frac{t_0}{2} = (1-t+\epsilon\frac{t_0}{2})\delta_n.$$

Thus for t in $[\epsilon t_0, t_0]$ the result follows. $\square$

Theorem 2.5 (Equioscillation)**.** *Suppose $l=0$ and K is compact. If the polynomial s_n^*, $n \geq 0$ is a solution of* (2.2)*, then there exist at least $n+2$ points $z_1,\dots,z_{n+2}$ in K such that*

$$\left|\frac{s_n^*(z_i)-f(z_i)}{s_n^*(z_i)+f(z_i)}\right| = \left\|\frac{s_n^*-f}{s_n^*+f}\right\|_\infty. \tag{2.5}$$

Proof. Let $z_1,\dots,z_m$ be all distinct points of equioscillation, *i.e* satisfying (2.5). We know that $m \geq 1$, since we maximize over a compact set. Now suppose that $m \leq n+1$ to reach a contradiction. First, we have $f(z_i) \neq 0$, since otherwise $\delta_n = 1$, which contradicts the result $\delta_n < 1$ from Theorem 2.2. We now use Lemma

2.4: we denote by $\mathcal{D}_i$ the disk with center z_i and radius ϵ_i defined in the lemma. By compactness, we have

$$\sup_{z\in K-(\bigcup \mathcal{D}_i)\cap K}\left|\frac{s_n^*(z)-f(z)}{s_n^*(z)+f(z)}\right| < \delta_n.$$

Then there exists a neighborhood U of s_n^* such that for any s in U,

$$\sup_{z\in K-(\bigcup \mathcal{D}_i)\cap K}\left|\frac{s(z)-f(z)}{s(z)+f(z)}\right| < \delta_n,$$

and in addition, because s is in the neighborhood U of s_n^*, we have by continuity

$$\sup_{z\in K}\left|\frac{s(z)-f(z)}{s(z)+f(z)}\right| = \sup_{z\in(\bigcup \mathcal{D}_i)\cap K}\left|\frac{s(z)-f(z)}{s(z)+f(z)}\right|.$$

For sufficiently small ϵ, by Lemma 2.4 there exists $t \in [\epsilon t_0, t_0]$ such that $s_n^* + ts$ is in U, and we have

$$\left\|\frac{s_n^*+ts-f}{s_n^*+ts+f}\right\|_\infty < \delta_n,$$

which is a contradiction, since we found a polynomial $s_n^* + ts$ which is a better approximation than s_n^* to f. □

Theorem 2.6 (Uniqueness)**.** *Suppose $l = 0$ and K compact. The solution s_n^* of* (2.2) *is unique for all $n \geq 0$.*

Proof. We first show that the set of best approximations is convex: let s_n^* and $\tilde{s}_n^*$ be two polynomials of best approximation, θ a real number between 0 and 1, and let $s = \theta s_n^* + (1-\theta)\tilde{s}_n^*$. Then for any z in K, $\frac{s_n^*}{f}(z)$ and $\frac{\tilde{s}_n^*}{f}(z)$ are contained in $\overline{\mathcal{D}}(1, \delta_n)$, which is a disk since $\delta_n < 1$, and hence convex. Thus for any z in K, $\frac{s}{f}(z)$ is also in $\overline{\mathcal{D}}(1, \delta_n)$, which means that $\left\|\frac{s-f}{s+f}\right\|_\infty \leq \delta_n$. Since δ_n is the infimum over all polynomials of degree n, we must have $\left\|\frac{s-f}{s+f}\right\|_\infty = \delta_n$ and s is therefore also a polynomial of best approximation: the set of best approximations is convex. Now we choose $n+2$ points $z_1, \ldots, z_{n+2}$ among the points of equioscillation of s. By definition $\frac{s}{f}(z_j)$ is on the boundary $\mathcal{C}(1, \delta_n)$ for all $j = 1, 2, \ldots, n+2$; but at the same time, $\frac{s_n^*}{f}(z_j)$ and $\frac{\tilde{s}_n^*}{f}(z_j)$ are in $\overline{\mathcal{D}}(1, \delta_n)$. The set $\overline{\mathcal{D}}(1, \delta_n)$ is, however, strictly convex, and thus a barycenter of two points can only be on the boundary if the points coincide,

$$\frac{s_n^*(z_j)}{f(z_j)} = \frac{\tilde{s}_n^*(z_j)}{f(z_j)} = \frac{s(z_j)}{f(z_j)}, \quad j = 1, 2, \ldots, n+2.$$

The difference $s_n^* - \tilde{s}_n^*$ therefore has at least $n+2$ roots, and since the polynomials are of degree at most n, they must coincide. □

Next we study local best approximations. We define a map on $\mathbf{P}_n$ by

$$h(s) = \left\|\frac{s-f}{s+f}\right\|_\infty, \quad s \in \mathbf{P}_n,$$

and we search for the local minima of h.

Theorem 2.7 (Local minima)**.** *Let s^* be a strict local minimum for h. Then s^* is the global minimum of h on $\mathbf{P}_n$.*

Proof. We introduce a family of closed subsets of $\mathbf{P}_n$ for any $\delta > 0$ by

$$\widetilde{\mathcal{D}}_\delta = \{s \in \mathbf{P}_n, \quad h(s) \leq \delta\}.$$

These sets fulfill several properties:

(i) For any $\delta < 1$, $\widetilde{\mathcal{D}}_\delta$ is a convex set. To see this, let s and $\tilde{s}$ be in $\widetilde{\mathcal{D}}_\delta$, and θ in $[0, 1]$. For any z in K, $\frac{s}{f}(z)$ and $\frac{\tilde{s}}{f}(z)$ are in $\mathcal{D}(1, \delta)$ which is convex by Lemma 2.1. Hence $\theta\frac{s}{f}(z) + (1-\theta)\frac{\tilde{s}}{f}(z)$ is in $\mathcal{D}(1, \delta)$, which implies that $\theta\frac{s}{f} + (1-\theta)\frac{\tilde{s}}{f}$ is in $\widetilde{\mathcal{D}}_\delta$.

(ii) The map $\delta \mapsto \widetilde{\mathcal{D}}_\delta$ is increasing, as one can infer directly from its definition.

We now conclude the proof of the theorem: let (s^*, δ^*) be a strict local minimum for h, and let (s^{**}, δ^{**}) be another local minimum, with $\delta^* \geq \delta^{**}$, and $s^* \neq s^{**}$. Then there exists a convex neighborhood U of s^*, such that for any s in U different from s^*, $h(s) > \delta^*$. Since $s^{**} \in \widetilde{\mathcal{D}}_{\delta^{**}} \subset \widetilde{\mathcal{D}}_{\delta^*}$, by the convexity of $\widetilde{\mathcal{D}}_{\delta^*}$, we have $[s^*, s^{**}] \subset \widetilde{\mathcal{D}}_{\delta^*}$. For ϵ small enough, we thus have $s_\epsilon = s^* + \epsilon(s^{**} - s^*)$ in $\widetilde{\mathcal{D}}_{\delta^*}$ and at the same time in U. This implies that $h(s_\epsilon) \leq \delta^*$ and at the same time $h(s_\epsilon) > \delta^*$, which is a contradiction. □

2.2. **Analysis of the case $l > 0$.** We now consider the best approximation problem (2.2) with a parameter $l > 0$, on a closed set K, not necessarily compact.

Theorem 2.8 (Existence)**.** *Let K be a closed set in $\mathbb{C}$, containing at least $n+2$ points. Let $f : K \to \mathbb{C}$ be a continuous function such that for every z in K, $\Re f(z) > 0$ and*

$$\Re f(z) \longrightarrow +\infty \text{ as } z \longrightarrow \infty \text{ in } K. \tag{2.6}$$

Then $\delta_n(l) < 1$ for all $n \geq 0$, and for l small enough, there exists a polynomial s_n^* solution to (2.2)*.*

Proof. By a standard compactness argument, property (2.6) implies that there exists $\alpha > 0$, such that for all $z \in K$, we have $\Re f(z) \geq \alpha > 0$. Now, $\left|\frac{1-f(z)}{1+f(z)}e^{-lf(z)}\right| \leq \left|\frac{1-f(z)}{1+f(z)}\right|e^{-l\alpha}$, and since $\Re f(z) > 0$, we have $\left|\frac{1-f(z)}{1+f(z)}\right| < 1$. Furthermore, $1 \in \mathbf{P}_n$ for all $n \geq 0$, which implies that

$$\delta_n(l) \leq \left\|\frac{1-f}{1+f}e^{-lf}\right\|_\infty \leq e^{-l\alpha} < 1,$$

which proves the first part of the theorem.

For the second part, let $(s_n^k)_{k\in\mathbb{N}}$ be a minimizing sequence. Then for all ϵ, there exists a k_0, such that for all $k \geq k_0$ we have

$$\delta_n(l) \leq \left\|\frac{s_n^k - f}{s_n^k + f}e^{-lf}\right\|_\infty \leq \delta_n(l) + \epsilon, \tag{2.7}$$

and if we choose $\epsilon \leq \frac{1-\delta_n(l)}{2}$, we have

$$\left\|\frac{s_n^k - f}{s_n^k + f}e^{-lf}\right\|_\infty \leq \frac{1+\delta_n(l)}{2} < 1.$$

Let $\beta > \alpha$ and $K_\beta = K \cap \{z, \alpha \leq \Re f(z) \leq \beta\}$. By property (2.6), K_β is a closed set, and for β large enough, it contains at least $n+2$ points. On this compact set, we obtain the estimate

$$\Big\|\frac{s_n^k-f}{s_n^k+f}\Big\|_{L^\infty(K_\beta)}=\Big\|\frac{s_n^k-f}{s_n^k+f}e^{-lf}e^{lf}\Big\|_{L^\infty(K_\beta)}\leq\Big\|\frac{s_n^k-f}{s_n^k+f}e^{-lf}\Big\|_{L^\infty(K_\beta)}e^{l\beta}\leq\frac{1+\delta_n(l)}{2}e^{l\beta},$$

and since $\frac{1+\delta_n(l)}{2}<1$, if l is such that $\frac{1+\delta_n(l)}{2}e^{l\beta}<1$, we get

$$\Big\|\frac{s_n^k-f}{s_n^k+f}\Big\|_{L^\infty(K_\beta)}<1,$$

which shows that the numerical sequence $\|s_n^k\|_{L^\infty(K_\beta)}$ is bounded. Since K_β contains at least $n+2$ points , $\|\cdot\|_{L^\infty(K_\beta)}$ induces a norm on the finite dimensional vector space $\mathbf{P}_n$. Hence a subsequence $s_n^{\phi(k)}$ converges to a s_n^* in $L^\infty(K_\beta)$. Since on $\mathbf{P}_n$ all norms are equivalent, for any z in K, $|\frac{s_n^*(z)-f(z)}{s_n^k(z)+f(z)}e^{-lf(z)}|=\lim_k|\frac{s_n^{\phi(k)}(z)-f(z)}{s_n^{\phi(k)}(z)+f(z)}e^{-lf(z)}|$, which is smaller than $\delta_n(l)+\epsilon$ for any ϵ by using (2.7). This proves the existence. □

The equioscillation property is shown as in the case $l=0$: we first have the results analogous to Lemma 2.3 and Lemma 2.4 (the proofs are identical):

Lemma 2.9. *Let the assumptions of Theorem 2.8 be verified. Then for a given vector $\boldsymbol{w}=(w_1,\dots,w_m)$, $m\leq n+1$, such that any w_i is in K and $w_i\neq w_j$ for $i\neq j$, the mapping*

$$\mathcal{A}_{\boldsymbol{w}}:U_{\boldsymbol{w}}\to\mathbb{C}^m,\quad s\mapsto\left(\frac{s(w_i)-f(w_i)}{s(w_i)+f(w_i)}e^{-lf(w_i)}\right)_{1\leq i\leq m}$$

is a submersion. Furthermore, its derivative with respect to s is continuous with respect to s and w.

Lemma 2.10. *Let s_n^* be a solution of (2.2) for $l>0$, and let $\boldsymbol{z}=(z_1,\dots,z_m)$ be a vector of m distinct points in K, $m\leq n+1$. We have*

(1) *s_n^* is in $U_{\boldsymbol{z}}$,*
(2) *let $\tilde{s}$ in $\mathbf{P}_n$ such that $\mathcal{A}'_{\boldsymbol{z}}(s_n^*)\ \tilde{s}=-\mathcal{A}_{\boldsymbol{z}}(s_n^*)$. Then for any $\epsilon>0$, there exist positive $(\epsilon_1,\dots,\epsilon_m)$, and $t_0\in]0,1[$, such that for any $t\in[\epsilon t_0,t_0]$ and for any z such that $|z-z_i|<\epsilon_i$ for some i,*

$$\left|\frac{s_n^*(z)+t\tilde{s}(z)-f(z)}{s_n^*(z)+t\tilde{s}(z)+f(z)}e^{-lf(z)}\right|\leq(1-\epsilon\frac{t_0}{2})\delta_n.$$

Theorem 2.11 (Equioscillation)**.** *With the assumptions of Theorem 2.8, if s_n^* is a solution of problem (2.2) for $l>0$, then there exist at least $n+2$ points $z_1,\dots,z_{n+2}$ in K such that*

$$\left|\frac{s_n^*(z_i)-f(z_i)}{s_n^*(z_i)+f(z_i)}e^{-lf(z_i)}\right|=\left\|\frac{s_n^*-f}{s_n^*+f}e^{-lf}\right\|_\infty.$$

Proof. Using the fact that

$$\delta_n(l)\leq\left\|\frac{s_n^*-f}{s_n^*+f}e^{-lf}\right\|_\infty\leq\delta_n e^{-l\inf_K\Re f}<1,$$

the proof of the theorem follows as in the case where $l=0$. □

To prove uniqueness in the general case, we need to assume the compactness of K:

Theorem 2.12 (Uniqueness). *With the assumptions of Theorem* 2.8*, if K is a compact set and l satisfies*

$$\delta_n(l)e^{l\sup_{z\in K}\Re f(z)} < 1, \tag{2.8}$$

then problem (2.2) *has a unique solution s_n^* for all $n \geq 0$.*

Proof. We first prove that the set of best approximations is convex: let s_n^* and $\tilde{s}_n^*$ be two polynomials of best approximation, θ in $[0,1]$ and let $s = \theta s_n^* + (1-\theta)\tilde{s}_n^*$. For any z in D, $\frac{s_n^*}{f}(z)$ and $\frac{\tilde{s}_n^*}{f}(z)$ are in $\overline{\mathcal{D}}(1, \delta_n(l)e^{l\Re f(z)})$, which is convex since

$$\delta_n e^{l\Re f(z)} \leq \delta_n e^{l\sup_K \Re f(z)} < 1$$

by condition (2.8). Thus for any z in K, $\frac{s}{f}(z)$ is in $\overline{\mathcal{D}}(1, \delta_n(l)e^{l\Re f(z)})$, which means that $\left\|\frac{s-f}{s+f}e^{-lf}\right\|_\infty \leq \delta_n(l)$. Since $\delta_n(l)$ is the infimum, we have $\left\|\frac{s-f}{s+f}e^{-lf}\right\|_\infty = \delta_n(l)$, and s is also a best approximation. The conclusion follows now as in the proof of Theorem 2.6. □

2.3. **The symmetric case.** Now we derive specific results for the best approximation problems arising in the context of waveform relaxation methods:

Definition 2.13. The symmetric case of the homographic best approximation problem (2.2) is the case where K is a closed set, symmetric with respect to the real axis, containing at least $n+2$ points, and for any z in K, $f(\bar{z}) = \overline{f(z)}$.

Theorem 2.14. *In the symmetric case of Definition* 2.13*, if K is a compact set and l is zero or sufficiently small in order to satisfy* (2.8)*, then the polynomial of best approximation s_n^* of f in K has real coefficients.*

Proof. If s_n^* is the polynomial of best approximation for f, we have

$$\begin{aligned}\sup\nolimits_K \left|\tfrac{s_n^*(z)-f(z)}{s_n^*(z)+f(z)}e^{-lf(z)}\right| &= \sup\nolimits_K \left|\tfrac{s_n^*(\bar{z})-f(\bar{z})}{s_n^*(\bar{z})+f(\bar{z})}e^{-lf(\bar{z})}\right| \\ &= \sup\nolimits_K \left|\tfrac{s_n^*(\bar{z})-\overline{f(z)}}{s_n^*(\bar{z})+\overline{f(z)}}e^{-l\overline{f(z)}}\right| = \sup\nolimits_K \left|\tfrac{\overline{s_n^*(\bar{z})}-f(z)}{\overline{s_n^*(\bar{z})}+f(z)}e^{-lf(z)}\right|,\end{aligned}$$

which shows that $\overline{s_n^*(\bar{z})} = s_n^*(z)$ for every z in K by uniqueness, and hence proves that s_n^* has real coefficients. □

We denote by τ the complex involution $z \mapsto \bar{z}$. From now on, K_1 is a closed set in the upper half-plane $\Im z \geq 0$, and $K = K_1 \cup \tau(K_1)$. We consider the minimization problem on K_1 restricted to the space $\mathbf{P}_n^r$ of polynomials with real coefficients, with the functional

$$h_l^r(s) = \left\|\frac{s-f}{s+f}e^{-lf}\right\|_{L^\infty(K_1)}, \tag{2.9}$$

and the real best approximation problem

$$\sup_{z\in K_1}\left|\frac{s_n^{r,*}(z)-f(z)}{s_n^{r,*}(z)+f(z)}e^{-lf(z)}\right| = \inf_{s\in\mathbf{P}_n^r}\sup_{z\in K_1}\left|\frac{s(z)-f(z)}{s(z)+f(z)}e^{-lf(z)}\right|. \tag{2.10}$$

Theorem 2.15. *In the symmetric case of Definition* 2.13*, suppose that K_1 is compact, l is zero or is sufficiently small to satisfy* (2.8)*. Then any strict local minimum of h_l^r in $\mathbf{P}_n^r$ is a global minimum in $\mathbf{P}_n^r$, and is unique.*

Proof. With condition (2.8), the proof is the same as in Theorem 2.7. □

Corollary 2.16. *Under the assumptions in Theorem* 2.15*, any strict local minimum of* h_l^r *in* $\mathbf{P}_n^r$ *is the global minimum for the complex best approximation problem* (2.2) *on* K.

Proof. By Theorem 2.14, the solution of the complex problem (2.2) is real, and is therefore a global minimum for h_l^r. But if there is a strict local minimum for h_l^r, it is the only global minimum of h_l^r, and therefore coincides with the solution of the complex problem (2.2). □

In the noncompact case, there is no such result available, but we will only need to solve a particular problem. We introduce the notation $\mathbf{P}_1^+ = \{s = p + qz, p \geq 0, q \geq 0\}$ and $\mathbb{C}^+ = \{z, \Re z \geq 0, \Im z \geq 0\}$ and consider the problem of finding $s_1^{+,*}$ in $\mathbf{P}_1^+$ such that

$$\sup_{z\in K_1}\left|\frac{s_1^{+,*}(z) - f(z)}{s_1^{+,*}(z) + f(z)}e^{-lf(z)}\right| = \inf_{s\in\mathbf{P}_1^+}\sup_{z\in K_1}\left|\frac{s(z) - f(z)}{s(z) + f(z)}e^{-lf(z)}\right|. \tag{2.11}$$

Theorem 2.17. *Suppose* $K_1 \subset \mathbb{C}^+$*, then any strict local minimum of* h_l^r *in* $\mathbf{P}_1^+$ *is a global minimum.*

Proof. The proof is an extension of the proof of Theorem 2.7. We introduce a family of subsets of $\mathbf{P}_1^+$ for any $\delta > 0$ by

$$\widetilde{\mathcal{D}}_\delta^l = \{s \in \mathbf{P}_1^+, h_l^r(s) \leq \delta\}.$$

The only difference compared to the proof of Theorem 2.7 is the proof of property (i), which states that for any $\delta < 1$, $\widetilde{\mathcal{D}}_\delta^l$ is a convex set. To show this, let s and $\tilde{s}$ be in $\widetilde{\mathcal{D}}_\delta^l$. For any z in K_1, $s(z)$ and $\tilde{s}(z)$ are in $\mathcal{D}(f(z), \delta e^{l\Re f(z)}) \cap \mathbb{C}^+$. If $\delta e^{l\Re f(z)} < 1$, $\mathcal{D}(f(z), \delta e^{l\Re f(z)})$ is convex by Lemma 2.1, whereas if $\delta e^{l\Re f(z)} \geq 1$, since $f(z) \in \mathbb{C}^+$, $\mathbb{C}^+ \subset \mathcal{D}(f(z), \delta e^{l\Re f(z)})$, and $\mathbb{C}^+ \cap \mathcal{D}(f(z), \delta e^{l\Re f(z)}) = \mathbb{C}^+$. In any case $\mathcal{D}(f(z), \delta e^{l\Re f(z)}) \cap \mathbb{C}^+$ is convex. Then, for any z in K_1, such that $\Im z > 0$, we have $\frac{1}{2}(s(z) + \tilde{s}(z))$ is in $\mathcal{D}(f(z), \delta e^{l\Re f(z)}) \cap \mathbb{C}^+$. Thus $\frac{1}{2}(s + \tilde{s})$ is in $\widetilde{\mathcal{D}}_\delta^l$ which proves the convexity, since $\widetilde{\mathcal{D}}_\delta^l$ is a closed set. Having established convexity, the result follows as in Theorem 2.7. □

Remark 2.18. It is tempting at this stage to believe that the number of equioscillation points for the real problem (2.10) or (2.11) is also $\geq n + 2$. We will prove in Section 4 that this is true for our special problem, when $n = 1$ and the size of K_1 is sufficiently large in $\mathbb{C}^+$. However, it is not true in general, and we will show a counterexample at the end of Section 4.1.1.

3. Model problem and Schwarz waveform relaxation algorithms

The homographic best approximation problem (2.1, 2.2) we studied in Section 2 is important for solving evolution problems in parallel. To define a parallel algorithm in space-time, Schwarz waveform relaxation algorithms use a decomposition of the spatial domain into subdomains, and then iteratively compute subdomain solutions in space-time, which are becoming better and better approximations to the solution on the whole space-time domain; see [22]. Our guiding example here is the advection reaction diffusion equation in $\mathbb{R}^N$,

$$\partial_t u + (\boldsymbol{a} \cdot \boldsymbol{\nabla})u - \nu\Delta u + bu = f.$$

The analysis we present here is for the decomposition into two half-spaces only, but our numerical experiments in Section 6 show that the theoretical results are also relevant for more than two subdomains. We define $\Omega = \mathbb{R} \times \mathbb{R}^{N-1}$ with coordinate $(x, \boldsymbol{y}) = (x, y_1, \ldots, y_{N-1})$, and use for the advection vector the notation $\boldsymbol{a} = (a, \boldsymbol{c})$, which leads to

$$\mathcal{L}u = \partial_t u + a\partial_x u + (\boldsymbol{c} \cdot \boldsymbol{\nabla_y})u - \nu\Delta u + bu = f, \quad \text{in } \Omega \times (0, T). \tag{3.1}$$

The diffusion coefficient ν is strictly positive, and we assume that a and b are constants which do not both vanish simultaneously. The case of the heat equation needs special treatment and can be found in [13]. Without loss of generality, we can assume that the advection coefficient a in the x direction is nonnegative, since $a < 0$ amounts to changing x into $-x$. We can also assume that the reaction coefficient b is nonnegative. If not, a change of variables $v = ue^{-\zeta t}$, with $\zeta + b > 0$ will lead to (3.1) with a positive reaction coefficient. We split $\Omega = \mathbb{R}^N$ into two subdomains $\Omega_1 = (-\infty, L) \times \mathbb{R}^{N-1}$ and $\Omega_2 = (0, \infty) \times \mathbb{R}^{N-1}$, $L \geq 0$. A Schwarz waveform relaxation algorithm then consists of solving iteratively subproblems on $\Omega_1 \times (0, T)$ and $\Omega_2 \times (0, T)$ using general transmission conditions at the interfaces $\Gamma_0 = \{0\} \times \mathbb{R}^{N-1}$ and $\Gamma_L = \{L\} \times \mathbb{R}^{N-1}$, i.e. defining a sequence (u_1^k, u_2^k), for $k \in \mathbb{N}$, such that

(3.2)
$$\begin{array}{rclrcl} \mathcal{L}u_1^k &=& f \quad \text{in } \Omega_1 \times (0,T), & \mathcal{L}u_2^k &=& f \quad \text{in } \Omega_2 \times (0,T), \\ u_1^k(\cdot,\cdot,0) &=& u_0 \quad \text{in } \Omega_1, & u_2^k(\cdot,\cdot,0) &=& u_0 \quad \text{in } \Omega_2, \\ \mathcal{B}_1 u_1^k &=& \mathcal{B}_1 u_2^{k-1} \text{ on } \Gamma_L \times (0,T), & \mathcal{B}_2 u_2^k &=& \mathcal{B}_2 u_1^{k-1} \text{ on } \Gamma_0 \times (0,T), \end{array}$$

where $\mathcal{B}_1$ and $\mathcal{B}_2$ are linear operators in space and time, possibly pseudo-differential, and an initial guess $\mathcal{B}_2 u_1^0(0, \cdot, \cdot)$ and $\mathcal{B}_1 u_2^0(L, \cdot, \cdot)$, $t \in (0, T)$, needs to be provided.

The classical Schwarz waveform relaxation algorithm is obtained by choosing $\mathcal{B}_1$ and $\mathcal{B}_2$ equal to the identity, as in the case of the Schwarz domain decomposition methods for elliptic problems [37, 30]. With this choice, the algorithm is convergent only with overlap. This algorithm has been studied in [15] and [31] for the present model problem; for earlier studies, see [21, 23, 22].

A better choice, which leads to faster algorithms, and can be convergent even without overlap, is

$$\mathcal{B}_j = \partial_x + \mathcal{S}_j(\boldsymbol{\nabla_y}, \partial_t), \quad j = 1, 2\,, \tag{3.3}$$

where the $\mathcal{S}_j$ are ordinary linear pseudo-differential operators in $(\boldsymbol{y}, t)$, related to their total symbols $\sigma_j(\boldsymbol{\eta}, \omega)$ by [25]

$$\mathcal{S}_j(\boldsymbol{\nabla_y}, \partial_t)u(\boldsymbol{y}, t) = (2\pi)^{-n/2} \int \sigma_j(\boldsymbol{\eta}, \omega)\hat{u}(\boldsymbol{\eta}, \omega)e^{i(\boldsymbol{\eta} \cdot \boldsymbol{y} + \omega t)}\, d\boldsymbol{\eta}\, d\omega.$$

The best operators $\mathcal{S}_j$ are related to transparent boundary operators, which have first been exploited in [4] for stationary problems, and in [17] for time dependent problems. They can be found by the following analysis. Let e_i^k be the error in Ω_i, i.e. $e_i^k = u_i^k - u$. Using a Fourier transform in time with parameter ω and in $\boldsymbol{y}$ with parameter $\boldsymbol{\eta}$, the Fourier transforms $\hat{e}_j^k$ in time and $\boldsymbol{y}$ of e_j^k are solutions of the ordinary differential equation in the x variable

$$-\nu\frac{\partial^2 \hat{e}}{\partial x^2} + a\frac{\partial \hat{e}}{\partial x} + \big(i(\omega + \boldsymbol{c} \cdot \boldsymbol{\eta}) + \nu|\boldsymbol{\eta}|^2 + b\big)\hat{e} = 0.$$

The characteristic roots are

$$r^+ = \frac{a+\sqrt{d}}{2\nu}, \quad r^- = \frac{a-\sqrt{d}}{2\nu}, \quad d = a^2 + 4\nu(i(\omega + \boldsymbol{c}\cdot\boldsymbol{\eta}) + \nu|\boldsymbol{\eta}|^2 + b).$$

The complex square root in this text is always with strictly positive real part. In order to work with at least square integrable functions in time and space, we look for solutions which do not increase exponentially in x. Since $\Re r^+ > 0$ and $\Re r^- < 0$, we obtain

$$\hat{e}_1^k(x,\boldsymbol{\eta},\omega) = \alpha_1^k(\boldsymbol{\eta},\omega)e^{r^+(x-L)}, \qquad \hat{e}_2^k(x,\boldsymbol{\eta},\omega) = \alpha_2^k(\boldsymbol{\eta},\omega)e^{r^-x}. \tag{3.4}$$

Inserting (3.4) into the transmission conditions (3.3), we find that for any $k \geq 2$,

$$\alpha_j^{k+1} = \rho\,\alpha_j^{k-1}, \quad j = 1, 2,$$

with the convergence factor

$$\rho = \frac{r^- + \sigma_1}{r^+ + \sigma_1}\cdot\frac{r^+ + \sigma_2}{r^- + \sigma_2}\; e^{(r^- - r^+)L}, \quad \forall\omega\in\mathbb{R},\ \boldsymbol{\eta}\in\mathbb{R}^{N-1}. \tag{3.5}$$

Hence, if the symbols σ_j are chosen to be

$$\sigma_1 = -r^-, \qquad \sigma_2 = -r^+, \tag{3.6}$$

then algorithm (3.2) converges in 2 steps, independently of the initial guess. This is an optimal result, since the solution on one subdomain necessarily depends on the right-hand side of function f on the other subdomain, and hence at least one communication is necessary for convergence. The choice in (3.6), however, leads to nonlocal operators $\mathcal{S}_j$, since r^+ and r^- are not polynomials in the dual variables, and nonlocal operators are less convenient to implement and more costly to use than local ones. It is therefore of interest to approximate the optimal choice σ_j in (3.6) corresponding to the optimal transmission operators by polynomials in $(\omega,\boldsymbol{\eta})$, which leads to differential operators $\mathcal{S}_j$. We suppose in the sequel that the $\mathcal{S}_j$, $j = 1, 2$, are chosen in a symmetric way, i.e. their symbols are of the form

$$\sigma_1 = \frac{-a+s}{2\nu}, \quad \sigma_2 = \frac{-a-s}{2\nu},$$

where s is a polynomial in the dual variables. Defining the complex function z of $(\omega,\boldsymbol{\eta})$ by

$$z = 4\nu\big(i(\omega + \boldsymbol{c}\cdot\boldsymbol{\eta}) + \nu|\boldsymbol{\eta}|^2\big), \tag{3.7}$$

we obtain for the convergence factor (3.5),

$$\rho(z,s) = \left(\frac{s(z) - \sqrt{a^2+4\nu b+z}}{s(z) + \sqrt{a^2+4\nu b+z}}\right)^2 e^{-\frac{L}{\nu}\sqrt{a^2+4\nu b+z}}. \tag{3.8}$$

In numerical computations, the frequencies ω and $\boldsymbol{\eta}$ are bounded, i.e. $|\omega| \leq \omega_{\max}$ and $|\eta_j| \leq \eta_{j,\max}$ where $\omega_{\max}$ is a discrete frequency which can be estimated by $\omega_{\max} = \pi/\Delta t$, where Δt is the time step, and similarly $\eta_{j,\max} = \pi/\Delta y_j$. In the nonoverlapping case, we define the compact set

$$K = \{z \in \mathbb{C}, |\omega| \leq \omega_{\max}, |\eta_j| \leq \eta_{j,\max}, j = 1,\dots,N-1\}.$$

In the overlapping case, we shall also consider $\omega_{\max} = \infty$ and $\eta_{j,\max} = \infty$, which leads to a noncompact set K.

For any integer n we search for s_n^* in $\mathbf{P}_n$, the complex space of polynomials of degree less than or equal to n with complex coefficients, such that

$$\sup_{z \in K} |\rho(z, s_n^*)| = \inf_{s \in \mathbf{P}_n} \sup_{z \in K} |\rho(z, s)|. \tag{3.9}$$

Problem (3.9) is a special case of (2.2) with

$$f(z) = \sqrt{\xi_0^2 + z}, \quad l = \frac{L}{2\nu}, \quad \xi_0 = \sqrt{a^2 + 4\nu b}, \tag{3.10}$$

and the assumptions on f in Section 2 are verified with $\Re f(z) \geq \xi_0 > 0$.

Next we focus on first order approximations, i.e. $s = p + qz$, which leads to first order optimized Schwarz waveform relaxation algorithms (3.2) with transmission conditions

(3.11)

$$\mathcal{S} = p + 4q\nu(\partial_t + (\boldsymbol{c} \cdot \boldsymbol{\nabla}_{\boldsymbol{y}}) - \nu\Delta_{\boldsymbol{y}}), \quad \mathcal{B}_1 = \partial_x - \frac{a}{2\nu} + \frac{1}{2\nu}\mathcal{S}, \quad \mathcal{B}_2 = \partial_x - \frac{a}{2\nu} - \frac{1}{2\nu}\mathcal{S}.$$

The case of zeroth order transmission conditions, $q = 0$, was studied in [15] for one-dimensional problems, and existence and convergence proofs together with numerical experiments were shown in [31] for two-dimensional problems. Using the general results from Section 2, we now solve the best approximation problem with first degree polynomials in one dimension.

4. Study and optimization of the convergence factor

We start with the one-dimensional case, for which the conditions of Section 2.3 hold, with $K_1 = i[0, \omega_{\max}]$. We proved in Theorem 2.14 that the polynomial of best approximation in the complex domain K has real coefficients, and we established in Corollary 2.16 the connection between the complex problem and the real problem, for $\omega_{\max} < +\infty$. In this section, we give more precise results on equioscillation properties for the real problem, in both the overlapping and nonoverlapping cases, which allows us to compute the optimal choice for the coefficients p and q in the optimized Schwarz waveform relaxation algorithm (3.2) with transmission conditions (3.11).

If $p, q \in \mathbb{R}$, then the modulus of the convergence factor (3.8) is

$$R(\xi, p, q, \xi_0, L) = \frac{(\xi - p)^2 + (\xi^2 - \xi_0^2)(2q\xi - 1)^2}{(\xi + p)^2 + (\xi^2 - \xi_0^2)(2q\xi + 1)^2} e^{-\frac{L}{\nu}\xi}, \tag{4.1}$$

where we have used the change of variables

$$\xi = \Re(\sqrt{a^2 + 4\nu(b + i\omega)}), \tag{4.2}$$

and $\xi_0 = \sqrt{a^2 + 4\nu b}$ from (3.10). We first propose and analyze a low frequency approximation for the first order transmission conditions, and then solve the best approximation problem, to derive optimized parameters p and q. In both cases, we analyze the performance of the overlapping ($L > 0$) and nonoverlapping case ($L = 0$).

4.1. **Low frequency approximation.** As a simple approach, a low frequency approximation of the optimal transmission conditions (3.6) can be used to determine the two parameters p and q. We call this case T1 for Taylor of order one. Using a Taylor expansion of the square root $\sqrt{a^2+4\nu(b+i\omega)}$ in (3.6) about $\omega=0$, we find

$$\sqrt{a^2+4\nu(b+i\omega)}=\sqrt{a^2+4\nu b}+\frac{2\nu}{\sqrt{a^2+4\nu b}}i\omega+O(\omega^2),$$

and hence for the parameters p and q the values

$$p=p_T=\sqrt{a^2+4\nu b} \quad \text{and} \quad q=q_T=\frac{1}{2\sqrt{a^2+4\nu b}}. \tag{4.3}$$

4.1.1. *The nonoverlapping case.* For $L=0$, $p=p_T$ and $q=q_T$, the convergence factor (4.1) becomes

$$R(\xi,p_T,q_T,\xi_0,0)=\left(\frac{\xi-\xi_0}{\xi+\xi_0}\right)^2. \tag{4.4}$$

The bound on the frequency parameter ω given before, $|\omega|\leq\omega_{\max}=\pi/\Delta t$, gives a bounded range $\xi_0\leq\xi\leq\xi_{\max}$, where

$$\xi_{\max}=\sqrt{\frac{\sqrt{\xi_0^4+16\nu^2\omega_{\max}^2}+\xi_0^2}{2}}. \tag{4.5}$$

Proposition 4.1 (T1 convergence factor estimate without overlap)**.** *The convergence factor in* (4.4) *is for* $\xi_0\leq\xi<\xi_{\max}$ *uniformly bounded by*

$$R_{T1}(\xi_0,\xi_{\max})=\left(\frac{\xi_{\max}-\xi_0}{\xi_{\max}+\xi_0}\right)^2. \tag{4.6}$$

For Δt *small, this maximum can be expanded as* $1-2\xi_0\sqrt{\frac{2}{\nu\pi}}\sqrt{\Delta t}+O(\Delta t)$.

Proof. Since $R(\xi,p_T,q_T,\xi_0,0)$ is a monotonically increasing function for $\xi\geq\xi_0$, the bound for $\xi_0\leq\xi\leq\xi_{\max}$ is attained at $\xi=\xi_{\max}$, which leads, using the variable transform (4.2) and $\omega_{\max}=\frac{\pi}{\Delta t}$ to the bound given in (4.6). ◻

Remark 4.2. The convergence factor estimate (4.6) for the first order Taylor transmission conditions is the square of the convergence factor estimate found in [15] for the zeroth order Taylor transmission conditions.

4.1.2. *The overlapping case.* With $L>0$, $p=p_T$ and $q=q_T$, and the change of variables (4.2), the convergence factor (4.1) becomes

$$R(\xi,p_T,q_T,\xi_0,L)=\left(\frac{\xi-\xi_0}{\xi+\xi_0}\right)^2 e^{-\frac{\xi L}{\nu}}. \tag{4.7}$$

We first present a convergence factor estimate for ω in $\mathbb{R}$.

Proposition 4.3 (T1 convergence factor estimate with overlap)**.** *The convergence factor in* (4.7) *satisfies*

$$\begin{aligned} R_{T1}^{\infty}(\xi_0,L)&=\max_{\xi_0\leq\xi<+\infty}R(\xi,p_T,q_T,\xi_0,L)\\ &=\left(\frac{\bar\xi-\xi_0}{\bar\xi+\xi_0}\right)^2 e^{-\frac{L\bar\xi}{\nu}},\ \textit{with}\ \bar\xi=\sqrt{\xi_0^2+\frac{4\nu\xi_0}{L}}. \end{aligned} \tag{4.8}$$

For L *small, this maximum can be expanded as* $1-4\sqrt{\frac{\xi_0}{\nu}}\sqrt{L}+O(L)$.

Proof. Taking a derivative of the convergence factor $R(\xi, p_T, q_T, \xi_0, L)$ defined in (4.7) with respect to ξ shows that there is a unique maximum for $\xi \geq \xi_0$ at $\xi = \bar{\xi}$ given in (4.8). Evaluating R for $\xi = \bar{\xi}$ and expanding for L small leads to the asymptotic result. □

In a numerical computation, the overlap L is in general not a fixed quantity; one can only afford that a few grid cells overlap, $L = C_1\Delta x$. In addition, there is also often a relation between the time and space step of the form $\Delta t = C_2\Delta x^\beta$, $\beta > 0$, due to accuracy or stability constraints. There exists a limiting value of the overlap, namely

$$L_1 = \frac{8\nu\xi_0}{\sqrt{\xi_0^4 + 16\nu\omega_{\max}} - \xi_0^2}, \tag{4.9}$$

such that for $L > L_1$, $\xi_{\max} > \bar{\xi}$, and hence the contraction factor in (4.8) is relevant. On the other hand, if $L \leq L_1$, then $\xi_{\max} \leq \bar{\xi}$ and hence numerically the contraction factor in (4.8) becomes irrelevant. Numerically, the relevant bound is therefore by monotonicity

$$\begin{aligned} R_{T1}(\xi_0, \xi_{\max}, L) &= \max_{\xi_0 \leq \xi \leq \xi_{\max}} R(\xi, p_T, q_T, \xi_0, L) \\ &= \begin{cases} R_{T1}^\infty(\xi_0, L), & \text{if } L > L_1, \\ \left(\frac{\xi_{\max}-\xi_0}{\xi_{\max}+\xi_0}\right)^2 e^{-\frac{L\xi_{\max}}{\nu}}, & \text{if } L \leq L_1. \end{cases} \end{aligned} \tag{4.10}$$

Proposition 4.4 (T1 discrete convergence factor estimate with overlap)**.** *If $L = C_1\Delta x$ and $\Delta t = C_2\Delta x^\beta$ with $\beta > 0$, then the bound in* (4.10) *on the convergence factor has for Δx small the expansion*

$$\begin{aligned} &R_{T1}(\xi_0, \xi_{\max}, L) \\ &= \begin{cases} 1 - 4\sqrt{\frac{C_1\xi_0}{\nu}}\sqrt{\Delta x} + O(\Delta x), & \textit{if } \beta > 1, \textit{ or } \beta = 1 \textit{ and } \frac{C_1}{C_2} > \frac{2\xi_0}{\pi}, \\ 1 - \frac{\sqrt{2}(2C_2\xi_0 + C_1\pi)}{\sqrt{C_2\pi\nu}}\sqrt{\Delta x} + O(\Delta x), & \textit{if } \beta = 1 \textit{ and } \frac{C_1}{C_2} \leq \frac{2\xi_0}{\pi}, \\ 1 - 2\xi_0\sqrt{\frac{2C_2}{\pi\nu}}\Delta x^{\frac{\beta}{2}} + o(\Delta x^{\frac{\beta}{2}}), & \textit{if } 0 < \beta < 1. \end{cases} \end{aligned} \tag{4.11}$$

Proof. Expanding (4.9) for Δt small, we obtain

$$L_1 = \frac{2\xi_0}{\pi}\Delta t + O(\Delta t^2),$$

and comparing with $L = C_1\Delta x$, using that $\Delta t = C_2\Delta x^\beta$, we obtain the first case in (4.11). For the second case, one can set $\beta = 1$ and directly expand the second case of (4.10) to find the result given. For the last case, the expansion of the exponential term gives

$$e^{-\frac{L\xi_{\max}}{\nu}} = 1 - C_1\sqrt{\frac{2\pi}{C_2\nu}}\Delta x^{1-\frac{\beta}{2}} + O(\Delta x^{2-\beta}),$$

and the coefficient in front of the exponential in (4.10) has the expansion

$$\frac{\xi_{\max} - \xi_0}{\xi_{\max} + \xi_0} = 1 - \xi_0\sqrt{\frac{2C_2}{\pi\nu}}\Delta x^{\frac{\beta}{2}} + O(\Delta x^\beta).$$

Hence the result follows. □

4.2. **Optimization of the convergence factor.** We now use the general results from Section 2 on the homographic best approximation problem to optimize the waveform relaxation algorithm with transmission conditions (3.11) for the overlapping and nonoverlapping case. We will call this case O1 for optimized of order one.

4.2.1. *The nonoverlapping case.* The domain of definition for $f(z) = \sqrt{\xi_0^2 + 4\nu z}$ with $z = i\omega$ is $K = i[0, \omega_{\max}] \cup -i[0, \omega_{\max}]$. By Theorems 2.2 and 2.6, the problem (3.9) in $\mathbf{P}_1$ has a unique solution $s_1^* = p^* + 4\nu i\omega q^*$. By Theorem 2.14, s_1^* has real coefficients. Therefore, (p^*, q^*) is the unique pair of real numbers such that

$$\inf_{p,q\in\mathbb{R}} \sup_{\xi_0\le\xi\le\xi_{\max}} R(\xi, p, q, \xi_0, 0) = \sup_{\xi_0\le\xi\le\xi_{\max}} R(\xi, p^*, q^*, \xi_0, 0), \tag{4.12}$$

and we denote by R_{O1} the maximum of the convergence factor,

$$R_{O1}(\xi_0, \xi_{\max}) = \sup_{\xi_0\le\xi\le\xi_{\max}} R(\xi, p^*, q^*, \xi_0, 0).$$

$R_{O1}(\xi_0, \xi_{\max})$ is equal to δ_1^2 with the notation from Section 2.

Lemma 4.5. *The solution (p^*, q^*) of the min-max problem (4.12) satisfies $p^* > 0$ and $q^* \ge 0$.*

Proof. Knowing from Theorem 2.2 that $\delta_1 < 1$, and taking $\xi = \xi_0$ in (4.1), we first see that $p^* > 0$. Now for positive p and q, we see in (4.1) that $R(\xi, p, q, \xi_0, 0) \le R(\xi, p, -q, \xi_0, 0)$, which proves that $q^* \ge 0$. □

Because of the symmetry of the domain K, $\left\|\frac{s_1^*-f}{s_1^*+f}\right\|$ equioscillates at least twice in $[0, \omega_{\max}]$. We show now that for sufficiently large $\omega_{\max}$, the solution actually equioscillates three times on $[0, \omega_{\max}]$, and we give implicit formulas for the solution p^* and q^*.

Theorem 4.6 (O1 convergence factor estimate without overlap)**.** *For $\xi_{\max}$ sufficiently large, the solution of (4.12) equioscillates three times, i.e. p^* and q^* are the unique solution of the system of equations*

$$R(\xi_0, p, q, \xi_0, 0) = R(\bar\xi(p, q), p, q, \xi_0, 0) = R(\xi_{\max}, p, q, \xi_0, 0) \tag{4.13}$$

where $\bar\xi(p, q)$ is the second of the three distinct ordered positive roots (for $p > (1 + \sqrt{2})\xi_0$) of the bi-cubic polynomial

$$\begin{aligned} P(\xi) &= 32q^3\xi^6 - 16q(-3qp + 4q^2\xi_0^2 + 1)\xi^4 \\ &\quad + (8q\xi_0^2 + 32q^3\xi_0^4 - 24qp^2 - 16q^2\xi_0^2 p + 8p)\xi^2 - 4(\xi_0 - p)(\xi_0 + p)(2q\xi_0^2 - p). \end{aligned} \tag{4.14}$$

The optimal parameters and the bound on the convergence factor, which is the common value $R_{O1}(\xi, \xi_0, \xi_{\max})$ in (4.13) at point $(p, q) = (p^*, q^*)$, have the expansions

$$p^* \sim \xi_0^{\frac{3}{4}} \xi_{\max}^{\frac{1}{4}}, \quad \hat q^* \sim \frac{1}{2\xi_0^{\frac{1}{4}}} \xi_{\max}^{-\frac{3}{4}}, \quad R_{O1}(\xi_0, \xi_{\max}) \sim 1 - 4\xi_0^{\frac{1}{4}} \xi_{\max}^{-\frac{1}{4}}. \tag{4.15}$$

Proof. We start this proof by studying the variation of R for fixed p and q: the polynomial P given in (4.14) is the numerator of the partial derivative of R with respect to ξ. Therefore its roots determine the extrema of R. Since P is a bi-cubic polynomial with real coefficients, it has one, two or three positive distinct real roots. In the first two cases, since $R(0, p, q, \xi_0, 0) = 1$, $R \le 1$ for $\xi \ge \xi_0$ and $R \longrightarrow 1$ as $\xi \longrightarrow \infty$, R reaches a unique minimum in $[\xi_0, \xi_{\max}]$, and therefore if $p = p^*$ and

$q = q^*$, R equioscillates at points ξ_0 and $\xi_{\max}$ only. If there are three ordered distinct positive real roots, then the second one, $\bar{\xi}$, must correspond to a maximum of R and the other ones to minima. The maximum of R can thus be attained at the local maximum at $\bar{\xi}$, or at the endpoints ξ_0 and $\xi_{\max}$.

We now focus on the condition for these three points to give equioscillations for R, i.e. on solving (4.13). We first prove that the equation $R(\xi_0, p, q, \xi_0, 0) = R(\xi_{\max}, p, q, \xi_0, 0)$ has, for any $p > (1+\sqrt{2})\xi_0$, two positive solutions, and we define a function $\hat{q}$ by $\hat{q}(p) = q$, the largest positive one. Then we prove in Lemma 4.7 that for $\xi_{\max}$ large and $q = \hat{q}(p)$, the polynomial P has precisely three distinct positive roots, and we estimate $\bar{\xi}(p, \hat{q}(p))$. After this step, we deduce in Lemma 4.8 that for $\xi_{\max}$ sufficiently large there is at least one solution p_* to

$$R(\xi_0, p, \hat{q}(p), \xi_0) = R(\bar{\xi}(p, \hat{q}(p)), p, \hat{q}(p), \xi_0). \tag{4.16}$$

We then expand $(p_*, q_* = \hat{q}(p_*))$ asymptotically as $\xi_{\max}$ tends to infinity, and we finally show that $s_1 = p_* + 4i\omega\nu q_*$ is a strict local minimum for h_l^r defined in (2.9), with $l = 0$, $K_1 = i[0, \omega_{\max}]$, and $n = 1$. Corollary 2.16 then states that $(p^*, q^*) = (p_*, q_*)$, which concludes the proof.

The equation $R(\xi_0, p, q, \xi_0, 0) = R(\xi_{\max}, p, q, \xi_0, 0)$ can be rewritten as an equation for the q variable,

(4.17)
$$-4p\xi_0(\xi_{\max}+\xi_0)\xi_{\max}^2 q^2 + 2(\xi_{\max}+\xi_0)(p^2+\xi_0^2)\xi_{\max} q + p(p^2 - 2\xi_0\xi_{\max} - \xi_0^2) = 0.$$

The discriminant of (4.17) is

$$\Delta = \xi_{\max}^2(\xi_{\max}+\xi_0)\big[\xi_{\max}(p^4 - 6\xi_0^2p^2 + \xi_0^4) + \xi_0\big((p^2-\xi_0^2)^2 + 4p^4\big)\big], \tag{4.18}$$

and is positive for large $\xi_{\max}$ under the assumption $p > (1+\sqrt{2})\xi_0$. Since the sum and the product of the roots in (4.17) is positive, there are two positive roots, and we choose $q = \hat{q}(p)$ as the larger one, i.e.[1]

(4.19)
$$\hat{q}(p) = \frac{(\xi_0^2+p^2)\sqrt{\xi_0+\xi_{\max}} + \sqrt{(5\xi_0+\xi_{\max})p^4 - 2\xi_0^2(\xi_0+3\xi_{\max})p^2 + \xi_0^4(\xi_0+\xi_{\max})}}{4p\xi_0\xi_{\max}\sqrt{\xi_0+\xi_{\max}}}.$$

Lemma 4.7. *Let p be any positive real number with $p > (1+\sqrt{2})\xi_0$, and let $q = \hat{q}(p)$ be defined in (4.19). Then for sufficiently large $\xi_{\max}$, the polynomial P in (4.14) has exactly three distinct real roots. As $\xi_{\max}$ tends to infinity, the first one has a limit equal to $\sqrt{(p^2-\xi_0^2)/2}$, the second one, $\bar{\xi}(p, \hat{q}(p))$, is equivalent to $\sqrt{p\xi_{\max}/2q_0}$, and the third one tends to infinity like $\xi_{\max}/\sqrt{2}q_0$, where q_0 depends on p and ξ_0, $q_0 = \big(\xi_0^2 + p^2 + \sqrt{p^4 - 6\xi_0^2p^2 + \xi_0^4}\big)/4p\xi_0$.*

Proof. From the formula for q in (4.19), we obtain that for fixed p, we have $q \sim \frac{q_0}{\xi_{\max}}$ as $\xi_{\max} \to +\infty$. We perform the change of variables $\chi = \xi^2/\xi_0\xi_{\max}$, which transforms the equation $P(\xi) = 0$ into $\tilde{P}(\chi) = 0$ with

$$\tilde{P}(\chi) \sim 32\xi_0^3q_0^3\chi^3 - 16q_0\xi_0^2(\xi_{\max} - 3q_0p)\chi^2 + 8\xi_0(p\xi_{\max} + q_0\xi_0^2 - 3q_0p^2)\chi + 4p(\xi_0^2 - p^2).$$

$\tilde{P}$ has three real roots. Using the sum of the roots, we see that the largest one tends to infinity like $\frac{\xi_{\max}}{2\xi_0q_0^2}$, then by the second symmetric function of the roots, the middle one tends to $\frac{p}{2\xi_0q_0}$, and finally usingthe product of the roots, the smallest

[1]Formula (4.19) together with (4.16) can be useful to compute the optimal parameters, since it reduces the problem to finding a root of a scalar equation.

one tends to zero like $\frac{p^2-\xi_0^2}{2\xi_0\xi_{\max}}$. From these expressions the result follows by inverting the change of variable. □

Lemma 4.8. *For $\xi_{\max}$ sufficiently large, there exists at least one solution $p_* > (1+\sqrt{2})\xi_0$ to* (4.16)*. Moreover, for any fixed p_0, if $\xi_{\max}$ is large, there is no solution in* $[0, p_0]$.

Proof. For any fixed p, we have that $R(\xi_0, p, \hat{q}(p), \xi_0, 0) < 1$ independently of $\xi_{\max}$, and $R(\bar{\xi}(p, \hat{q}(p)), p, \hat{q}(p), \xi_0, 0)$ tends to 1 as $\xi_{\max}$ tends to infinity. Therefore, for $\xi_{\max}$ large, $R(\xi_0, p, \hat{q}(p), \xi_0, 0) - R(\bar{\xi}(p, \hat{q}(p)), p, \hat{q}(p), \xi_0, 0)$ is negative for any fixed p. If p tends to infinity, we have

$$R(\xi_0, p, \hat{q}(p), \xi_0, 0) = \left(\frac{p-\xi_0}{p+\xi_0}\right)^2 \sim 1 - 4\xi_0/p \quad \text{independently of } \xi_{\max}. \tag{4.20}$$

On the other hand, for $\xi_{\max}$ large and fixed, if p tends to infinity, we have

$$R(\bar{\xi}(p, \hat{q}(p)), p, \hat{q}(p), \xi_0, 0) \sim \left(\frac{p-\bar{\xi}}{p+\bar{\xi}}\right)^2 \sim 1 - 4\frac{\bar{\xi}}{p}. \tag{4.21}$$

Since $\bar{\xi} > \xi_0$, $R(\xi_0, p, \hat{q}(p), \xi_0, 0) - R(\bar{\xi}(p, \hat{q}(p)), p, \hat{q}(p), \xi_0, 0)$ becomes positive for large p. By continuity, there exist a p_* for which this expression vanishes. □

We now expand p_* and $\hat{q}(p_*)$ asymptotically: by Lemma 4.8, p_* tends to infinity with $\xi_{\max}$. Hence we can use (4.20), (4.21). Using the formula for $q = \hat{q}(p)$ in (4.19), we have that for $\xi_{\max}$, as p tends to infinity, $\hat{q}(p) \sim p/2\xi_0\xi_{\max}$ and $\bar{\xi}(p, \hat{q}(p)) \sim \sqrt{\xi_0\xi_{\max}}$. Therefore, in order to match the two expansions in (4.20), (4.21), p has to tend to infinity more slowly than $\sqrt{\xi_0\xi_{\max}}$, which gives $p_* \sim \xi_0^{3/4}\xi_{\max}^{1/4}$. Inserting this into (4.19) leads to $q_* = \hat{q}(p_*) \sim \frac{1}{2\xi_0^{\frac{1}{4}}}\xi_{\max}^{-\frac{3}{4}}$. Finally, inserting p_* and q_* into $R(\xi_0, p_*, q_*, \xi_0, 0)$ and expanding for $\xi_{\max}$ we obtain

$$R(\xi_0, p_*, q_*, \xi_0, 0) \sim 1 - 4\frac{\xi_0}{p} \sim 1 - 4\xi_0^{\frac{1}{4}}\xi_{\max}^{-\frac{1}{4}}. \tag{4.22}$$

Lemma 4.9. *$s_1 = p_* + 4\nu i\omega q_*$ is a strict local minimum for h_0^r in $\mathbf{P}_1^r$, with $K_1 = i[0, \omega_{\max}]$.*

Proof. For any (p, q), we define $r = \frac{1}{q}$ and

$$\mu(p, q, \xi_0, \xi_{\max}) = \sup_{\xi \in [\xi_0, \xi_{\max}]} \frac{1 + R(\xi, p, q, \xi_0, 0)}{1 - R(\xi, p, q, \xi_0, 0)},$$

and write

$$R(\xi, p, q, \xi_0, 0) - \sup_{\xi \in [\xi_0, \xi_{\max}]} R(\xi, p, q, \xi_0, 0) = 4q^2 \frac{Q(\xi, p, r, \mu)}{(\xi+p)^2 + (\xi^2 - \xi_0^2)(2\xi q + 1)^2},$$

with

$$Q(\xi, p, r, \mu) = \xi^4 - \mu r \xi^3 + (\frac{r^2}{2} - \xi_0^2)\xi^2 + \mu r(\xi_0^2 - \frac{pr}{2})\xi + r^2\frac{p^2 - \xi_0^2}{4}.$$

In what follows, we will consider Q as a polynomial in the independent variables ξ, p, r and μ. $(p_*, r_*, \mu_* = \mu(p_*, q_*, \xi_0, \xi_{\max}))$ is a solution of the system of equations

$$Q(\xi_0, p_*, r_*, \mu_*) = 0, \;\; Q(\xi_{\max}, p_*, r_*, \mu_*) = 0, \;\; Q(\bar{\xi}, p_*, r_*, \mu_*) = \partial_\xi Q(\bar{\xi}, p_*, r_*, \mu_*) = 0.$$

Now for s_1 to be a strict local minimum for h_0^r, it is sufficient that there exists no variation $(\delta p, \delta r, \delta\mu)$ with $\delta\mu < 0$, such that $Q(\xi, p_*+\delta p, r_*+\delta r, \mu_*+\delta\mu) < 0$ for $\xi = \xi_0, \bar{\xi}$ and $\xi_{\max}$. By Taylor's formula, it suffices to prove this for $\delta p \frac{\partial Q}{\partial p}(\xi, p_*, r_*, \mu_*) + \delta r \frac{\partial Q}{\partial r}(\xi, p_*, r_*, \mu_*) + \delta\mu \frac{\partial Q}{\partial \mu}(\xi, p_*, r_*, \mu_*)$. Expanding the arguments of Q for $\xi_{\max}$ large, we have from the asymptotic results (4.22) the leading order terms. Including the next higher order terms, we obtain

$$
\begin{aligned}
\bar{\xi}(p_*, q_*) &= \xi_0^{\frac{1}{2}} \xi_{\max}^{\frac{1}{2}} (1 + \tfrac{1}{2} \xi_0^{\frac{1}{2}} \xi_{\max}^{-\frac{1}{2}} + o(\xi_{\max}^{-\frac{1}{2}})),\\
p_* &= \xi_0^{\frac{3}{4}} \xi_{\max}^{\frac{1}{4}} (1 + \tfrac{1}{4} \xi_0^{\frac{1}{2}} \xi_{\max}^{-\frac{1}{2}} + o(\xi_{\max}^{-\frac{1}{2}})),\\
r_* &= 2\xi_0^{\frac{1}{4}} \xi_{\max}^{\frac{3}{4}} (1 + \tfrac{3}{4} \xi_0^{\frac{1}{2}} \xi_{\max}^{-\frac{1}{2}} + o(\xi_{\max}^{-\frac{1}{2}})),\\
\mu_* &= \tfrac{1}{2}\xi_0^{-\frac{1}{4}} \xi_{\max}^{\frac{1}{4}} (1 + \tfrac{5}{4} \xi_0^{\frac{1}{2}} \xi_{\max}^{-\frac{1}{2}} + o(\xi_{\max}^{-\frac{1}{2}})),
\end{aligned}
\tag{4.23}
$$

where the expansion is best obtained using the elementary symmetric functions of the roots, and then identifying terms in the expansions. The partial derivatives of Q are

$$
\begin{aligned}
\frac{\partial Q}{\partial p} &= \frac{r^2}{2}(p - \mu\xi),\\
\frac{\partial Q}{\partial r} &= -\mu\xi^3 + r\xi^2 + \mu(\xi_0^2 - pr)\xi + \frac{rp^2}{2},\\
\frac{\partial Q}{\partial \mu} &= -r\xi^3 + r(\xi_0^2 - \frac{pr}{2})\xi.
\end{aligned}
\tag{4.24}
$$

Inserting the expansions (4.23) into (4.24), we obtain for the expansions of the partial derivatives

$$
\begin{array}{llll}
\frac{\partial Q}{\partial p} \sim \xi_0^{\frac{5}{4}} \xi_{\max}^{\frac{7}{4}}, & \frac{\partial Q}{\partial r} \sim -\frac{1}{2}\xi_0^{\frac{11}{4}} \xi_{\max}^{\frac{1}{4}}, & \frac{\partial Q}{\partial \mu} \sim -2\xi_0^{\frac{9}{4}} \xi_{\max}^{\frac{7}{4}}, & \text{for } \xi = \xi_0,\\
\frac{\partial Q}{\partial p} \sim -\xi_0^{\frac{3}{4}} \xi_{\max}^{\frac{9}{4}}, & \frac{\partial Q}{\partial r} \sim +\frac{1}{2}\xi_0^{\frac{5}{4}} \xi_{\max}^{\frac{7}{4}}, & \frac{\partial Q}{\partial \mu} \sim -4\xi_0^{\frac{7}{4}} \xi_{\max}^{\frac{9}{4}}, & \text{for } \xi = \bar{\xi},\\
\frac{\partial Q}{\partial p} \sim -\xi_0^{\frac{1}{4}} \xi_{\max}^{\frac{11}{4}}, & \frac{\partial Q}{\partial r} \sim -\frac{1}{2}\xi_0^{-\frac{1}{4}} \xi_{\max}^{\frac{13}{4}}, & \frac{\partial Q}{\partial \mu} \sim -2\xi_0^{\frac{1}{4}} \xi_{\max}^{\frac{15}{4}}, & \text{for } \xi = \xi_{\max}.
\end{array}
\tag{4.25}
$$

Let $(\delta p, \delta r, \delta\mu)$ such that $\delta p \frac{\partial Q}{\partial p}(\xi, p_*, r_*, \mu_*) + \delta r \frac{\partial Q}{\partial r}(\xi, p_*, r_*, \mu_*) + \delta\mu \frac{\partial Q}{\partial \mu}(\xi, p_*, r_*, \mu_*) < 0$ for $\xi = \xi_0$, $\xi = \bar{\xi}$ and $\xi = \xi_{\max}$. Using the expansion (4.25), we have for large $\xi_{\max}$,

$$
\begin{aligned}
\xi_{\max}^{\frac{3}{2}} \delta p - \tfrac{1}{2}\xi_0^{\frac{3}{2}} \delta r - 2\xi_0 \xi_{\max}^{\frac{3}{2}} \delta\mu &< 0,\\
-\xi_{\max}^{\frac{1}{2}} \delta p + \tfrac{1}{2}\xi_0^{\frac{1}{2}} \delta r - 4\xi_0 \xi_{\max}^{\frac{1}{2}} \delta\mu &< 0,\\
-\xi_0^{\frac{1}{2}} \delta p - \tfrac{1}{2}\xi_{\max}^{\frac{1}{2}} \delta r - 2\xi_0^{\frac{1}{2}} \xi_{\max} \delta\mu &< 0.
\end{aligned}
\tag{4.26}
$$

For $\delta\mu < 0$, equations (4.26) imply

$$
\left(\frac{\xi_{\max}}{\xi_0}\right)^{\frac{3}{2}} \delta p - \frac{1}{2}\delta r < 0, \qquad -\left(\frac{\xi_{\max}}{\xi_0}\right)^{\frac{1}{2}} \delta p + \frac{1}{2}\delta r < 0, \qquad -\delta p - \frac{1}{2}\left(\frac{\xi_{\max}}{\xi_0}\right)^{\frac{1}{2}} \delta r < 0.
\tag{4.27}
$$

Adding the first two inequalities in (4.27) yields $((\frac{\xi_{\max}}{\xi_0})^{\frac{3}{2}} - (\frac{\xi_{\max}}{\xi_0})^{\frac{1}{2}})\delta p < 0$, which implies $\delta p < 0$. From the second inequality we then obtain $\delta r < 0$, which together contradict the last inequality in (4.27). □

By Corollary 2.16, we obtain $(p_*, q_*) = (p^*, q^*)$, which concludes the proof of Theorem 4.6. □

If the algorithm is discretized in time with a time step Δt, then $\xi_{\max}$ is indeed large for $\Delta t \to 0$ and we obtain from (4.15):

Corollary 4.10 (O1 discrete convergence factor estimate without overlap)**.** *For Δt small, there is a unique solution of the min-max problem* (4.12)*. The values of p^*, q^* and $R_{O1}(\xi_0, \xi_{\max})$ have the following asymptotic leading order term as Δt tends to* 0*:*

$$p^* \sim \xi_0^{\frac{3}{4}} (2\pi\nu)^{\frac{1}{8}} \Delta t^{-\frac{1}{8}},\ q^* \sim \frac{1}{2\xi_0^{\frac{1}{4}}(2\pi\nu)^{\frac{3}{8}}} \Delta t^{\frac{3}{8}},\ R_{O1}(\xi_0, \xi_{\max}) \sim 1 - 4\xi_0^{\frac{1}{4}}(2\pi\nu)^{-\frac{1}{8}} \Delta t^{\frac{1}{8}}.$$

Remark 4.11. In the course of Theorem 4.6, we have proved the first assertion in Remark 2.18: for large $\omega_{\max}$, which corresponds to large K_1, the number of equioscillation points for the real problem (2.10) is actually equal to 3. For the second assertion in that remark, we show now that, when $\omega_{\max}$ tends to 0, or equivalently $\xi_{\max}$ tends to ξ_0, there cannot be three equioscillations points for the best approximation polynomial s_1^*. Suppose there are three equioscillation points. The study of R in the first part of the proof of Theorem 4.6 shows that two of them have to be ξ_0 and $\xi_{\max}$. Letting $\xi_{\max} = \xi_0(1 + \epsilon)$, with $\epsilon > 0$, we first see that p^* has to tend to ξ_0 with $\xi_{\max}$. On the one hand, we have

$$h(s_1^*) \le h(\xi_0) = \frac{\xi_{\max} - \xi_0}{\xi_{\max} + \xi_0} \sim \frac{\epsilon}{2}.$$

and on the other hand,

$$h(s_1^*) \ge \left| \frac{f(0) - s_1^*(0)}{f(0) + s_1^*(0)} \right| = \left| \frac{p^* - \xi_0}{p^* + \xi_0} \right|,$$

which proves that p^* tends to ξ_0. Therefore, it has the form $p^* = \xi_0(1 + C\epsilon) + \mathcal{O}(\epsilon^2)$ with $C \le 1$. Inserting these values into the formula for the discriminant in (4.18) gives $\Delta \sim 8\xi_0^8(2C - 1)\epsilon$, which implies $C \ge 1/2$. We now calculate from (4.19) $q^* \sim \frac{1}{2\xi_0}$. For $p = \xi_0$ and $q = \frac{1}{2\xi_0}$, the polynomial P is equal to $\frac{4}{\xi_0^3}\xi^4(\xi^2 - \xi_0^2)$, which has ξ_0 as a root. This shows that there is an extremum at ξ_0, but it is a minimum of R, since the derivative of P with respect to ξ is equal to $8\xi_0^2 > 0$.

4.2.2. *The overlapping case.* With the exponential weight, it is interesting to consider first the best approximation problem for ω in $\mathbb{R}$, since this gives insight for the discrete case with limiting value $\omega_{\max}$. With the notation in Section 2, this corresponds to $l > 0$, $K_1 = i\mathbb{R}_+$, $K = i\mathbb{R}$. By Theorem 2.8, we know that a solution exists, but we lose the uniqueness and the fact that the coefficients are real. We therefore restrict our analysis to problem (2.11), and will use the *ad hoc* Theorem 2.17 to prove similar results as in the nonoverlapping case. With the notation in (4.1) and (4.2), problem (2.11) is equivalent to finding (p_∞^*, q_∞^*) in $(\mathbb{R}_+)^2$ such that

$$\inf_{p \ge 0, q \ge 0} \sup_{\xi \ge \xi_0} R(\xi, p, q, \xi_0, L) = \sup_{\xi \ge \xi_0} R(\xi, p_\infty^*, q_\infty^*, \xi_0, L). \tag{4.28}$$

We denote the value of the infimum as $R_{O1}^{\infty}(\xi_0, L)$. To simplify the notation, we set

$$\zeta = \frac{L\xi}{\nu}, \quad \zeta_0 = \frac{L\xi_0}{\nu}, \quad \tilde{p} = \frac{Lp}{\nu}, \quad \tilde{q} = \frac{\nu q}{L},$$

so we remove the explicit dependence on the overlap parameter L and the parameter ν of the convergence factor R given in (4.1). The value of R in the new variables ζ, $\tilde{p}$, $\tilde{q}$ and ζ_0, is

$$\tilde{R}(\zeta, \tilde{p}, \tilde{q}, \zeta_0) = R(\xi, p, q, \xi_0, L) = \frac{(\zeta - \tilde{p})^2 + (\zeta^2 - \zeta_0^2)(1 - 2\zeta\tilde{q})^2}{(\zeta + \tilde{p})^2 + (\zeta^2 - \zeta_0^2)(1 + 2\zeta\tilde{q})^2} e^{-\zeta}. \tag{4.29}$$

The new real best approximation problem is therefore to find $(\tilde{p}^*_\infty, \tilde{q}^*_\infty)$ in $(\mathbb{R}_+)^2$ such that

$$\inf_{\tilde{p}\geq 0,\tilde{q}\geq 0} \sup_{\zeta\geq\zeta_0} \tilde{R}(\zeta,\tilde{p},\tilde{q},\zeta_0) = \sup_{\zeta\geq\zeta_0} \tilde{R}(\zeta,\tilde{p}^*_\infty,\tilde{q}^*_\infty,\zeta_0). \tag{4.30}$$

We now show that, for small overlap L, there is a unique solution, which equioscillates at three points, and we obtain the analogue of Theorem 4.6.

Theorem 4.12 (O1 convergence factor estimate with overlap)**.** *For L sufficiently small, the solution of* (4.30) *is unique and equioscillates three times, i.e.* $(\tilde{p}^*_\infty, \tilde{q}^*_\infty)$ *is the unique solution of*

$$\tilde{R}(\zeta_0,\tilde{p},\tilde{q},\zeta_0) = \tilde{R}(\zeta_2(\tilde{p},\tilde{q}),\tilde{p},\tilde{q},\zeta_0) = \tilde{R}(\zeta_4(\tilde{p},\tilde{q}),\tilde{p},\tilde{q},\zeta_0) \tag{4.31}$$

where $\zeta_2(\tilde{p},\tilde{q})$ denotes the second and $\zeta_4(\tilde{p},\tilde{q})$ the fourth of the four distinct positive roots, ordered in increasing order, of the polynomial

(4.32)
$$\begin{aligned}P(\zeta) = {}&16\tilde{q}^4\zeta^8 - 32\tilde{q}^3(\tilde{q}\zeta_0^2+1)\zeta^6\\ &+(16\tilde{q} - 48\tilde{q}^2\tilde{p} + 16\tilde{q}^4\zeta_0^4 + 4 + 64\tilde{q}^3\zeta_0^2 + 8\tilde{q}^2\tilde{p}^2 + 8\tilde{q}^2\zeta_0^2 - 16\tilde{q}\tilde{p})\zeta^4\\ &+(16\tilde{q}\zeta_0^2\tilde{p} - 32\tilde{q}^3\zeta_0^4 - 8\tilde{q}\zeta_0^2 + 24\tilde{q}\tilde{p}^2 - 4\zeta_0^2 - 8\tilde{p} + 16\tilde{q}^2\zeta_0^2\tilde{p} - 8\tilde{q}^2\zeta_0^4 - 8\tilde{q}^2\zeta_0^2\tilde{p}^2)\zeta^2\\ &+(\zeta_0^2 - \tilde{p}^2)(\zeta_0^2 + 8\tilde{q}\zeta_0^2 - \tilde{p}^2 - 4\tilde{p}).\end{aligned}$$

For L small, the optimal parameters and the bound $R^\infty_{O1}(\xi_0, L)$ on the convergence factor, which is the common value in (4.31) *at point $(\tilde{p},\tilde{q}) = (\tilde{p}^*_\infty,\tilde{q}^*_\infty)$, have the expansion*

$$p^*_\infty \sim \xi_0^{\frac{4}{5}}\nu^{\frac{1}{5}}L^{-\frac{1}{5}}, \quad q^*_\infty \sim \frac{1}{2}\nu^{-\frac{3}{5}}\xi_0^{-\frac{2}{5}}L^{\frac{3}{5}}, \quad R^\infty_{O1}(\xi_0,L) \sim 1 - 4\xi_0^{\frac{1}{5}}\nu^{-\frac{1}{5}}L^{\frac{1}{5}}. \tag{4.33}$$

Proof. We first examine the variations of $\tilde{R}$. For fixed $\tilde{p},\tilde{q}$, the partial derivative of $\tilde{R}$ with respect to ζ shows that the roots of P given in (4.32) determine the extrema of $\tilde{R}$. Since P is a bi-quartic in ζ with real coefficients, it has at most four positive real roots, and hence for $\zeta \geq \zeta_0 \geq 0$, $\tilde{R}$ can have at most two interior maxima. Using the change of variables $\chi = 2\tilde{q}\zeta^2$, we obtain

$$\begin{aligned}P(\zeta) = {}&\chi^4 - 4\chi^3 + \left(\frac{4}{\tilde{q}} - 12\tilde{p} - 4\frac{\tilde{p}}{\tilde{q}} + 2\tilde{p}^2 + \frac{1}{\tilde{q}^2}\right)\chi^2 + \left(12\tilde{p}^2 - 4\frac{\tilde{p}}{\tilde{q}}\right)\chi + \tilde{p}^2(\tilde{p}^2+4\tilde{p})\\ &+\zeta_0^2\left[-4\tilde{q}\chi^3 + (2+16\tilde{q})\chi^2 + \left(8\tilde{q}\tilde{p} - 4\tilde{q}\tilde{p}^2 - \frac{2}{\tilde{q}} - 4 + 8\tilde{p}\right)\chi - 2\tilde{p}(\tilde{p} + 4\tilde{q}\tilde{p} + 2)\right]\\ &+\zeta_0^4\left[4\tilde{q}^2\chi^2 - 4\tilde{q}(1+4\tilde{q})\chi + 1 + 8\tilde{q}\right].\end{aligned}$$

The dominant part of P for $\tilde{q}$ sufficiently large, $\tilde{p}\tilde{q}$ sufficiently small, and for ζ_0 sufficiently small, is

$$P_0(\chi) = \chi^4 - 4\chi^3 + \frac{4}{\tilde{q}}\chi^2 - \frac{4\tilde{p}}{\tilde{q}}\chi + 4\tilde{p}^3.$$

This polynomial has four real positive distinct roots χ_j, $j = 1 \ldots 4$, ordered in increasing order. If $1/\tilde{q}$ and $\tilde{p}\tilde{q}$ tend to 0, we have $\chi_1 \sim \tilde{q}\tilde{p}^2$, $\chi_2 \sim \tilde{p}$, $\chi_3 \sim 1/\tilde{q}$, $\chi_4 \sim 4$. By a perturbation argument, it follows that for ζ_0 sufficiently small (which corresponds to L going to zero), P has 4 real positive distinct roots as well, with the asymptotic behavior

$$\zeta_1 \sim \frac{\tilde{p}}{\sqrt{2}}, \quad \zeta_2 \sim \sqrt{\frac{\tilde{p}}{2\tilde{q}}}, \quad \zeta_3 \sim \frac{1}{\tilde{q}\sqrt{2}}, \quad \zeta_4 \sim \frac{\sqrt{2}}{\tilde{q}}.$$

We now show that (4.31) has a solution $(\tilde{p}_*, \tilde{q}_*)$ for ζ_0 small. We add the assumptions that $\zeta_0 = o(\tilde{p})$ as $\tilde{p}$ tends to 0, and we easily find asymptotic expansions of the three terms in (4.31),

$$\begin{aligned} R_0 &= \tilde{R}(\zeta_0, \tilde{p}, \tilde{q}, \zeta_0) &&\sim 1 - 4\frac{\zeta_0}{\tilde{p}}, \\ R_2 &= \tilde{R}(\zeta_2(\tilde{p}, \tilde{q}), \tilde{p}, \tilde{q}, \zeta_0) &&\sim 1 - 4\sqrt{2\tilde{p}\tilde{q}}, \\ R_4 &= \tilde{R}(\zeta_4(\tilde{p}, \tilde{q}), \tilde{p}, \tilde{q}, \zeta_0) &&\sim 1 - 2\sqrt{\frac{2}{\tilde{q}}}. \end{aligned} \tag{4.34}$$

The map $(\tilde{p}, \tilde{q}) \mapsto (R_2 - R_0, R_4 - R_0)$ maps a domain $(q_0 < \tilde{q} < \tilde{p}/2\zeta_0^2, 0 < \tilde{p}\tilde{q} < \epsilon_0)$ for q_0 large and ϵ_0 small, onto a neighborhood of 0 in $\mathbb{R}^2$.

We now establish the asymptotic expansions for $(\tilde{p}_*, \tilde{q}_*)$. They are easily found by equating the expansions in (4.34). We solve

$$\frac{\zeta_0}{\tilde{p}} = \sqrt{2\tilde{p}\tilde{q}} = \frac{1}{\sqrt{2\tilde{q}}},$$

from which we deduce

$$\tilde{p}_* \sim \zeta_0^{4/5}, \quad \tilde{q}_* \sim \frac{1}{2}\zeta_0^{-2/5}, \tag{4.35}$$

and (4.33) by the change of variables. In particular, the assumption $\zeta_0 = o(\tilde{p})$ is validated.

We now prove that for L sufficiently small, $(\tilde{p}_*, \tilde{q}_*)$ is a strict local minimum for the best approximation problem (4.30). The pair $(\tilde{p}_*, \tilde{q}_*)$ is a strict local minimum if there exists no variation $(\delta p, \delta q)$ such that $\tilde{R}(\zeta, \tilde{p}_* + \delta p, \tilde{q}_* + \delta q, \zeta_0) < \tilde{R}(\zeta, \tilde{p}_*, \tilde{q}_*, \zeta_0)$ for $\zeta = \zeta_0, \zeta_2, \zeta_4$. By the Taylor formula, it suffices to prove that there is no variation $(\delta p, \delta q)$, such that $\delta p \frac{\partial \tilde{R}}{\partial p}(\zeta, \tilde{p}_*, \tilde{q}_*, \zeta_0) + \delta q \frac{\partial \tilde{R}}{\partial q}(\zeta, \tilde{p}_*, \tilde{q}_*, \zeta_0) < 0$ for $\zeta = \zeta_0, \zeta_2, \zeta_4$. For ζ_0 small, expanding the arguments of $\tilde{R}$, we have from (4.2.2) and (4.35) the leading order terms in the expansion. Including the next higher order terms, we find

$$\begin{aligned} \tilde{p}_* &\sim \zeta_0^{\frac{4}{5}}(1 - \tfrac{1}{15}\zeta_0^{\frac{2}{5}}), \qquad & \tilde{q}_* &\sim \tfrac{1}{2}\zeta_0^{-\frac{2}{5}}(1 - \tfrac{7}{10}\zeta_0^{\frac{2}{5}}), \\ \zeta_2 &\sim \zeta_0^{\frac{3}{5}}(1 + \tfrac{2}{15}\zeta_0^{\frac{2}{5}}), \qquad & \zeta_4 &\sim 2\zeta_0^{\frac{1}{5}}(1 + \tfrac{1}{10}\zeta_0^{\frac{2}{5}}). \end{aligned}$$

Inserting these expansions into the expressions of the derivatives of $\tilde{R}$, we get

$$\begin{aligned} \tfrac{\partial \tilde{R}}{\partial p}(\zeta_0, \tilde{p}_*, \tilde{q}_*, \zeta_0) &\sim 4\zeta_0^{\frac{3}{5}}, \qquad & \tfrac{\partial \tilde{R}}{\partial q}(\zeta_0, \tilde{p}_*, \tilde{q}_*, \zeta_0) &= 0, \\ \tfrac{\partial \tilde{R}}{\partial p}(\zeta_2, \tilde{p}_*, \tilde{q}_*, \zeta_0) &\sim -2\zeta_0^{\frac{3}{5}}, \qquad & \tfrac{\partial \tilde{R}}{\partial q}(\zeta_2, \tilde{p}_*, \tilde{q}_*, \zeta_0) &\sim -4\zeta_0^{\frac{3}{5}}, \\ \tfrac{\partial \tilde{R}}{\partial p}(\zeta_4, \tilde{p}_*, \tilde{q}_*, \zeta_0) &\sim -\tfrac{1}{2}\zeta_0^{\frac{1}{5}}, \qquad & \tfrac{\partial \tilde{R}}{\partial q}(\zeta_4, \tilde{p}_*, \tilde{q}_*, \zeta_0) &\sim 4\zeta_0^{\frac{3}{5}}. \end{aligned} \tag{4.36}$$

Let $\mathcal{E}$ be the set of vectors $(\delta p, \delta q)$ such that $\delta p \frac{\partial \tilde{R}}{\partial p}(\zeta, \tilde{p}_*, \tilde{q}_*, \zeta_0) + \delta q \frac{\partial \tilde{R}}{\partial q}(\zeta, \tilde{p}_*, \tilde{q}_*, \zeta_0) < 0$ for $\zeta = \zeta_0, \zeta_2, \zeta_4$. We need to prove that $\mathcal{E}$ is empty. For small ζ_0, $\mathcal{E}$ can be obtained using the expansion (4.36):

$$4\zeta_0^{\frac{3}{5}}\delta p < 0, \quad -2\zeta_0^{\frac{3}{5}}\delta p - 4\zeta_0^{\frac{3}{5}}\delta q < 0, \quad -\frac{1}{2}\zeta_0^{\frac{1}{5}}\delta p + 4\zeta_0^{\frac{3}{5}}\delta q < 0. \tag{4.37}$$

The first inequality in (4.37) implies $\delta p < 0$, while adding the second and the third inequality in (4.37) yields $\delta p > 0$, which is a contradiction, and thus the set $\mathcal{E}$ is empty.

Using the uniqueness in Theorem 2.17, we obtain $(\tilde{p}^*_\infty, \tilde{q}^*_\infty) = (\tilde{p}_*, \tilde{q}_*)$, which concludes the proof. □

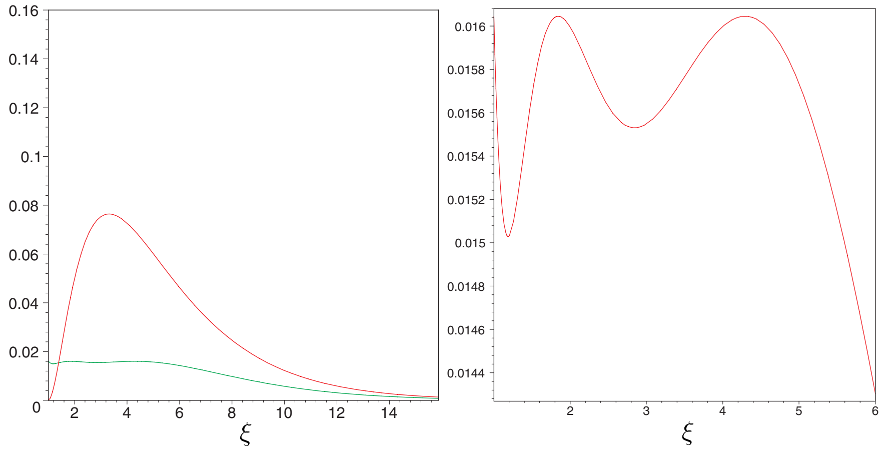

FIGURE 2. Convergence factors $R(\xi, p_T, q_T, \xi_0, L)$ (top curve) and $R(\xi, p_\infty^*, q_\infty^*, \xi_0, L)$ (curve below) for an overlapping example from the numerical section on the left, and zoom on $[0, 5]$ showing the equioscillation at the optimal solution on the right.

We show the convergence factors $R(\xi, p_T, q_T, \xi_0, L)$ and $R(\xi, p_\infty^*, q_\infty^*, \xi_0, L)$ in Figure 2 as functions of ξ for an example with $\xi_0 = 1$, $L = 0.08$ and $\nu = 0.2$ from the numerical section. One can see on the left the much better performance of the optimized first order transmission conditions compared to the first order Taylor transmission conditions, and also the equioscillation of the optimal choice on the right, which makes the convergence factor rather small and flat, before the effects of the exponential take over.

Theorem 4.12 gives the parameters p_∞^* and q_∞^* to choose in the first order transmission conditions of the optimized Schwarz waveform relaxation algorithm at the continuous level to get the best convergence factor, which is $1 - O(L^{\frac{1}{5}})$, and therefore is significantly better than the best result achievable with optimized Robin conditions [15], which led to a convergence factor $1 - O(L^{\frac{1}{3}})$.

In Figure 3, we show the first few iterations, at the end of the time interval, of the classical and optimized Schwarz waveform relaxation algorithm with first order optimized transmission conditions according to Theorem 4.12 for a model problem. This experiment shows well that the new transmission conditions improve the convergence behavior tremendously, they are very effective to transport the convected solution from left to right across the artificial interfaces between subdomains.

As we have seen earlier, in a numerical setting, not all the frequencies are present. We thus have to replace problem (4.29) by the min-max problem on the bounded domain $(\xi_0, \xi_{\max})$, which addresses the question if the maximum of the convergence factor attained at ξ_4 is relevant in a computation. Letting $L = C_1 \Delta x$ and $\Delta t = C_2 \Delta x^\beta$, the maximum numerical frequency we can expect on the time discretization grid leads from (4.5) to a bound on ζ, $\zeta_0 \leq \zeta \leq \zeta_{\max}$, where $\zeta_{\max}$ has the expansion

$$\zeta_{\max} = \frac{L x_{\max}}{\nu} = C_1 \Delta x \sqrt{\frac{\sqrt{x_0^4 + \left(\frac{4\nu\pi}{C_2 \Delta x^\beta}\right)^2} + x_0^2}{2}} = C_1 \sqrt{\frac{2\pi}{\nu C_2}} \Delta x^{1-\frac{\beta}{2}} + O(\Delta x^{1+\frac{\beta}{2}}).$$

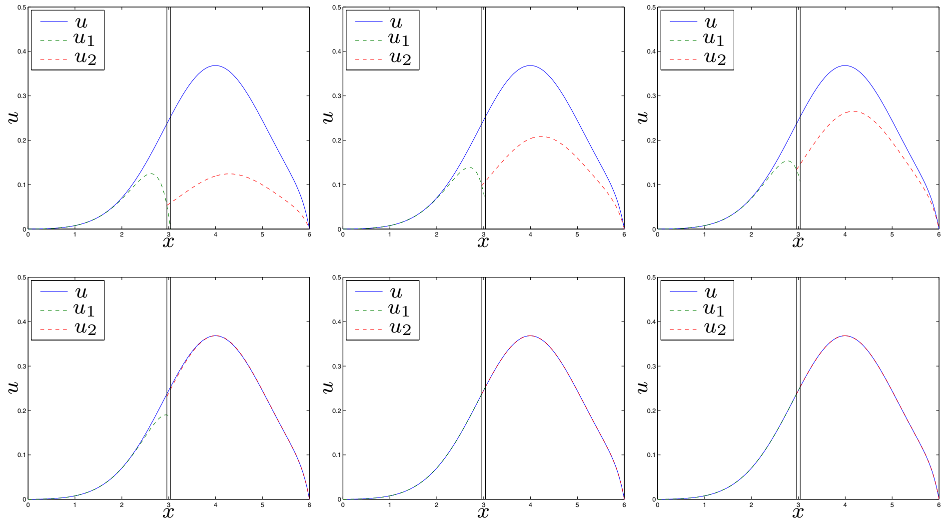

FIGURE 3. From left to right, the iterates $u_1^k(x,T)$ and $u_2^{k+1}(x,T)$ (dashed) at the end of the time interval $t = T$ for $k = 1, 3, 5$ for an example from the numerical section, together with the exact solution (solid). Top row the classical Schwarz waveform relaxation algorithm, and bottom row the optimized one.

Now ζ_4 from the optimization in (4.31) satisfies for L (and thus ζ_0) small

$$\zeta_4 \sim 2\zeta_0^{\frac{1}{5}} = 2\left(\frac{\xi_0 C_1}{\nu}\right)^{\frac{1}{5}} \Delta x^{\frac{1}{5}}.$$

Hence, if $1 - \frac{\beta}{2} = \frac{1}{5}$ i.e., $\beta = \frac{8}{5}$ and if C_1 is equal to the critical value $C_c = \nu^{\frac{3}{8}}\xi_0^{\frac{1}{4}}\left(\frac{2C_2}{\pi}\right)^{\frac{5}{8}}$, the numerical $\zeta_{\max}$ and ζ_4 from the optimization are asymptotically at the same location. This represents the boundary between the usefulness of the continuous optimization result (4.31) on an unbounded domain, and the optimization on the compact set $[0, \omega_{\max}]$. For the latter, the analysis in Section 2.2 becomes relevant, as we now show: by Theorems 2.8 and 2.12, problem (3.9) in $\mathbf{P}_1$ has a unique solution $s_1^* = p^* + 4i\omega\nu q^*$ for sufficiently small overlap L. By Theorem 2.14, s_1^* has real coefficients. Therefore, (p^*, q^*) is the unique pair of real numbers such that

$$\inf_{p,q\in\mathbb{R}} \sup_{\xi_0\le\xi\le\xi_{\max}} R(\xi, p, q, \xi_0, L) = \sup_{\xi_0\le\xi\le\xi_{\max}} R(\xi, p^*, q^*, \xi_0, L), \tag{4.38}$$

where we denote the infimum by $R_{O1}(\xi_0, \xi_{\max}, L)$, which is also equal to $\left(\delta_1(\frac{L}{2\nu})\right)^2$.

Lemma 4.13. *The solution* (p^*, q^*) *of the min-max problem* (4.38) *satisfies* $p^* > 0$ *and* $q^* \ge 0$.

Proof. By Theorems 2.2, 2.6 and 2.14, there is a unique real number p_0^* in $\mathbf{P}_0$ such that

$$\inf_{p\in\mathbb{R}} \sup_{\xi_0\le\xi\le\xi_{\max}} R(\xi, p, 0, \xi_0, 0) = \sup_{\xi_0\le\xi\le\xi_{\max}} R(\xi, p_0^*, 0, \xi_0, 0),$$

and the value of the infimum is δ_0^2. Furthermore, since $\delta_0 < 1$, p_0^* is positive. If (p^*, q^*) is a solution of the min-max problem (4.30), we have

$$\begin{aligned} R(\xi_0, p^*, q^*, \xi_0, L) = \frac{(\xi_0 - p^*)^2}{(\xi_0 + p^*)^2} e^{-\frac{L}{\nu}\xi_0} &\le \max_{\xi_0 \le \xi \le \xi_{\max}} R(\xi, p^*, q^*, \xi_0, L) \\ &\le \max_{\xi_0 \le \xi \le \xi_{\max}} R(\xi, p_0^*, 0, \xi_0, L) \le \max_{\xi_0 \le \xi \le \xi_{\max}} R(\xi, p_0^*, 0, \xi_0, 0) e^{-\frac{L}{\nu}\xi_0} \\ &\le \delta_0^2 e^{-\frac{L}{\nu}\xi_0} < e^{-\frac{L}{\nu}\xi_0}, \end{aligned}$$

with the notation from (2.1), which can only hold if $p^* > 0$. To prove that $q^* \ge 0$, we note that for negative q, we have for any $\xi \ge \xi_0$ from (4.1) $R(\xi, p, q, \xi_0, L) \ge R(\xi, p, -q, \xi_0, L)$, which can be seen by expanding the numerator of $R(\xi, p, q, \xi_0, L) - R(\xi, p, -q, \xi_0, L)$. □

Theorem 4.14 (O1 discrete convergence factor estimate with overlap)**.** *If $L = C_1 \Delta x$ and $\Delta t = C_2 \Delta x^\beta$, for Δx sufficiently small, we have the following asymptotic behaviors:*

(1) *For $\beta > \frac{8}{5}$, or $\beta = \frac{8}{5}$ and $C_1 > C_c$,*

$$R_{O1}(\xi_0, \xi_{\max}, L) \sim 1 - 4\left(\frac{C_1 \xi_0}{\nu}\right)^{\frac{1}{5}} \Delta x^{\frac{1}{5}},\ p^* \sim \left(\frac{\xi_0^4 \nu}{C_1}\right)^{\frac{1}{5}} \Delta x^{-\frac{1}{5}},\ q^* \sim 2 C_1^{\frac{3}{5}} \left(\frac{\nu}{\xi_0}\right)^{\frac{2}{5}} \Delta x^{\frac{3}{5}},$$

where $C_c = \nu^{\frac{3}{8}} \xi_0^{\frac{1}{4}} \left(\frac{2C_2}{\pi}\right)^{\frac{5}{8}}$.

(2) *For $\beta = \frac{8}{5}$ and $C_1 \le C_c$,*

$$R_{O1}(\xi_0, \xi_{\max}, L) \sim 1 - \left(\frac{4 C_1 \xi_0}{\tilde{C}_p \nu}\right) \Delta x^{\frac{1}{5}},\ p^* \sim \frac{\tilde{C}_p \nu}{C_1} \Delta x^{-\frac{1}{5}},\ q^* \sim 2 \frac{\xi_0^2 C_1^3}{\tilde{C}_p^3 \nu^2} \Delta x^{\frac{3}{5}},$$

where $\tilde{C}_p$ is the unique positive root of the polynomial

$$\tilde{P}(\xi) = 2\nu^3 C_2 \xi^4 + C_1 \pi \xi_0^2 \xi - 2\xi_0^3 C_1^4 \sqrt{\frac{2\pi C_2}{\nu}}.$$

(3) *Finally, for $0 < \beta < \frac{8}{5}$, we have*

$$R_{O1}(\xi_0, \xi_{\max}, L) \sim 1 - 2\left(\frac{2^7 C_2 \xi_0^2}{\pi \nu}\right)^{\frac{1}{8}} \Delta x^{\frac{\beta}{8}},\ p^* \sim \left(\frac{2\pi\nu\xi_0^6}{C_2}\right)^{\frac{1}{8}} \Delta x^{-\frac{\beta}{8}},\ q^* \sim \left(\frac{(2\nu)^5 C_2^3}{\xi_0^2 \pi^3}\right)^{\frac{1}{8}} \Delta x^{\frac{3\beta}{8}}.$$

Proof. We use here the notation introduced for Theorem 4.12 (see (4.29)) and consider the min-max problem in the form

$$\inf_{\tilde{p} \in \mathbb{R}, \tilde{q} \in \mathbb{R}} \sup_{\zeta_0 \le \zeta \le \zeta_{\max}} \tilde{R}(\zeta, \tilde{p}, \tilde{q}, \zeta_0) = \sup_{\zeta_0 \le \zeta \le \zeta_{\max}} \tilde{R}(\zeta, \tilde{p}^*, \tilde{q}^*, \zeta_0). \tag{4.39}$$

The proof of the first case is a direct consequence of Theorem 4.12 for the non-compact case with optimal parameters $(\tilde{p}_\infty^*, \tilde{q}_\infty^*)$, since in the first case, $\zeta_{\max} > \zeta_4(\tilde{p}_\infty^*, \tilde{q}_\infty^*)$.

For the two other cases, we have asymptotically $\zeta_3(\tilde{p}_\infty^*, \tilde{q}_\infty^*) \le \zeta_{\max} \le \zeta_4(\tilde{p}_\infty^*, \tilde{q}_\infty^*)$, and the proof follows the same steps as before: we first show the existence of $(\tilde{p}_*, \tilde{q}_*)$, such that $\tilde{R}(\zeta, \tilde{p}, \tilde{q}, \zeta_0)$ equioscillates at the three points ζ_0, $\zeta_2(\tilde{p}, \tilde{q})$ and $\zeta_{\max}$. We then determine the expansions of $(\tilde{p}_*, \tilde{q}_*)$, $\zeta_2(\tilde{p}_*, \tilde{q}_*)$, deduce that $(\tilde{p}_*, \tilde{q}_*)$ is a strict local minimum for h_l in $\mathbf{P}_n^r$, and finally conclude that $(\tilde{p}_*, \tilde{q}_*) = (\tilde{p}^*, \tilde{q}^*)$.

We work with ζ_0 as the small parameter: let $C_m = C_1\big(\frac{2\pi}{\nu C_2}\big)^{1/2}\big(\frac{\nu}{C_1\xi_0}\big)^{1-\beta/2}$, so that $\zeta_{\max} \sim C_m\zeta_0^{1-\beta/2}$. To prove the second and third result of the theorem, we need to study solutions of

$$\tilde{R}(\zeta_0, \tilde{p}, \tilde{q}, \zeta_0) = \tilde{R}(\zeta_2(\tilde{p}, \tilde{q}), \tilde{p}, \tilde{q}, \zeta_0) = \tilde{R}(\zeta_0, \tilde{p}, \tilde{q}, \zeta_{\max}) \tag{4.40}$$

for ζ_0 small. Let $R_0 := \tilde{R}(\zeta_0, \tilde{p}, \tilde{q}, \zeta_0)$, $R_2 := \tilde{R}(\zeta_2(\tilde{p}, \tilde{q}), \tilde{p}, \tilde{q}, \zeta_0)$ and $R_{\max} := \tilde{R}(\zeta_0, \tilde{p}, \tilde{q}, \zeta_{\max})$. A direct computation gives for $\tilde{q}$ large, and $\tilde{p}\tilde{q}$ and ζ_0 small,

$$R_{\max} \sim 1 - 4\left[\frac{1}{2q\zeta_{\max}} + \frac{\zeta_{\max}}{4}\right] \sim 1 - 4\left[\frac{1}{2q}\frac{\zeta_0^{\beta/2-1}}{C_m} + \frac{C_m\,\zeta_0^{1-\beta/2}}{4}\right].$$

Using the expansions from (4.34),

$$R_0 \sim 1 - 4\frac{\zeta_0}{\tilde{p}}, \quad R_2 \sim 1 - 4\sqrt{2\tilde{p}\tilde{q}},$$

we see first, by the Implicit Function Theorem, as in the proof of Theorem 4.12, that there exists a solution $(\tilde{p}_*, \tilde{q}_*)$ to (4.40). We find their behavior at infinity by equaling R_0, R_2 and $R_{\max}$, which gives the system of equations

$$C_m\zeta_0^{4-\beta/2} \sim \frac{C_m^2}{4}\tilde{p}\zeta_0^{4-\beta} + \tilde{p}^4, \quad \tilde{q} \sim \frac{\zeta_0^2}{2\tilde{p}^3}.$$

For $\beta = 8/5$, the two terms on the right in the first equation are balanced, which leads to $\tilde{p}_* \sim C\zeta_0^{4/5}$, where C is the unique positive root[2] of $C_m = (C^3 + C_m^2/4)C$ and $\tilde{q}_* \sim \frac{1}{2C^2}\zeta_0^{-2/5}$. For $\beta < 8/5$, the dominant term is $\tilde{p}^4$, from which we find $\tilde{p}_* \sim C_m^{1/4}\zeta_0^{1-\beta/2}$. Using the second equation, we obtain $\tilde{q}_* \sim \frac{1}{2}C_m^{-3/4}\zeta_0^{-1+\frac{3\beta}{8}}$. We now expand the partial derivatives of $\tilde{R}$ to show that, for L sufficiently small, $(\tilde{p}_*, \tilde{q}_*)$ is a strict local minimum for the best approximation problem (4.39). For R_0, we obtain, since ζ_0 is negligible with respect to p,

$$\frac{\partial\tilde{R}}{\partial\tilde{p}}(\zeta_0, \tilde{p}_*, \tilde{q}_*, \zeta_0) \sim 4C_m^{-1/2}\zeta_0^{-1+\beta/4}, \quad \frac{\partial\tilde{R}}{\partial\tilde{q}}(\zeta_0, \tilde{p}_*, \tilde{q}_*, \zeta_0) = 0.$$

For R_2, we use that $\zeta_0 \ll \tilde{p}_* \ll \zeta_2 \ll \zeta_{\max}$, and $\zeta_2\tilde{q}_* \sim \frac{1}{2}C_m^{-1/4}\zeta_0^{\beta/8}$, to obtain

$$\frac{\partial\tilde{R}}{\partial\tilde{p}}(\zeta_2, \tilde{p}_*, \tilde{q}_*, \zeta_0) \sim -2C_m^{-1/2}\zeta_0^{-1+\beta/4}, \quad \frac{\partial\tilde{R}}{\partial\tilde{q}}(\zeta_2, \tilde{p}_*, \tilde{q}_*, \zeta_0) \sim -2C_m^{1/2}\zeta_0^{1-\beta/4}.$$

For $R_{\max}$, we use $\zeta_{\max}\tilde{q}_* \sim \frac{C'}{2}\zeta_0^{-\beta/8}$ with $C' = C_m^{1/4}$ for $\beta < 8/5$ and $C' = C_m/C^2$ for $\beta = 8/5$,

$$\frac{\partial\tilde{R}}{\partial p}(\zeta_{\max}, \tilde{p}_*, \tilde{q}_*, \zeta_0) \sim -\zeta_{\max}^{-3}\tilde{q}_*^{-2} \sim -4C_m^{-1}C'^{-2}\zeta_0^{-1+3\beta/4},$$
$$\frac{\partial\tilde{R}}{\partial q}(\zeta_{\max}, \tilde{p}_*, \tilde{q}_*, \zeta_0) \sim 2\zeta_{\max}^{-1}\tilde{q}_*^{-2} \sim 8C_mC'^{-2}\zeta_0^{1-\beta/4}.$$

[2] This is a polynomial equation of fourth degree which is actually the first fourth degree equation which has been solved by Lodovico Ferrari in 1545. Note that all equations in the text result in polynomials of degree at most 4, and as such can be solved by radicals, using Del Ferro/Tartaglia/Cardan formulas [3].

After proceeding as in the proof of Theorem 4.12, we use Corollary 2.16 to conclude that $(\tilde{p}^*, \tilde{q}^*) = (\tilde{p}_*, \tilde{q}_*)$, and we have the asymptotic expansion

$$R_{O1}(\xi_0, \xi_{\max}, L) \sim 1 - 4\frac{\zeta_0^{\beta/2}}{C_m^{1/4}}.$$

Finally, note that for any $0 < \beta < 8/5$, the five extremal points of $\tilde{R}(\zeta, \tilde{p}_*, \tilde{q}_*, \zeta_0)$ behave as follows:

$$\zeta_0,\ \zeta_1 \sim \frac{C_m^{1/4}}{\sqrt{2}}\zeta_0^{1-\beta/8},\ \zeta_2 \sim C_m^{1/2}\zeta_0^{1-\beta/4},\ \zeta_3 \sim \sqrt{2}C_m^{3/4}\zeta_0^{1-3\beta/8},\ \zeta_{\max} \sim C_m\zeta_0^{1-\beta/2},$$

□

4.3. **Summary and extension to higher dimensions.** To summarize the results of this section, and to permit an easy search of the parameters p and q to be used in practice, we show in Table 1 an overview of the performance one can obtain with the various choices of the parameter p and q in the transmission conditions (3.11) of the new Schwarz waveform relaxation algorithm in one dimension.

TABLE 1. Summary of the asymptotic convergence factors for the parameter choices in the first order transmission conditions in one dimension, for $\Delta t = \Delta x^\beta$.

method	R	parameter p and q
Taylor no overlap	$1 - O(\sqrt{\Delta t})$	$\begin{cases} p = \sqrt{a^2+4\nu b} \\ q = \frac{2\nu}{\sqrt{a^2+4\nu b}} \end{cases}$
Optimized no overlap	$1 - O(\Delta t^{\frac{1}{8}})$	$\begin{cases} p = (2\nu\pi(a^2+4\nu b)^3)^{\frac{1}{8}}\Delta t^{-\frac{1}{8}} \\ q = (\pi^3(a^2+4\nu b))^{-\frac{1}{8}}(2\nu)^{\frac{5}{8}}\Delta t^{\frac{3}{8}} \end{cases}$
Taylor overlap Δx, $\beta \geq 1$	$1 - O(\sqrt{\Delta x})$	$\begin{cases} p = \sqrt{a^2+4\nu b} \\ q = \frac{2\nu}{\sqrt{a^2+4\nu b}} \end{cases}$
Taylor overlap Δx, $\beta < 1$	$1 - O(\Delta x^{\frac{\beta}{2}})$	
Optimized overlap Δx, $\beta > \frac{8}{5}$	$1 - O(\Delta x^{\frac{1}{5}})$	$\begin{cases} p = (\nu(a^2+4\nu b)^2)^{\frac{1}{5}}\Delta x^{-\frac{1}{5}} \\ q = 2\nu^{\frac{2}{5}}(a^2+4\nu b)^{-\frac{1}{5}}\Delta x^{\frac{3}{5}} \end{cases}$
Optimized overlap Δx, $\beta < \frac{8}{5}$	$1 - O(\Delta x^{\frac{\beta}{8}})$	$\begin{cases} p = (2\nu\pi(a^2+4\nu b)^3)^{\frac{1}{8}}\Delta x^{-\frac{\beta}{8}} \\ q = (2\nu)^{\frac{5}{8}}(\pi^3(a^2+4\nu b))^{-\frac{1}{8}}\Delta x^{\frac{3\beta}{8}} \end{cases}$

In higher dimension, without showing the details of the derivation, the Taylor transmission conditions lead to the parameters $p_T = \sqrt{a^2+4\nu b}$ and $q_T = \frac{2\nu}{\sqrt{a^2+4\nu b}}$ with associated convergence factor $1 - O(\Delta x)$ in the case without overlap, and $1 - O(\sqrt{\Delta x})$ in the case with overlap $O(\Delta x)$. Even if we do not have the complete analysis in this general case for the optimized problem (i.e. the equivalent of Theorems 4.6, 4.12 and Corollary 4.10), we can still give formally the order of magnitude of the various quantities. The optimal parameters in the transmission conditions are for the nonoverlapping case asymptotically given by $p = C_p\Delta x^{-\frac{1}{4}}$ and $q = C_q\Delta x^{\frac{3}{4}}$, which leads to an optimized convergence factor $1 - O(\Delta x^{\frac{1}{4}})$ of the associated optimized Schwarz waveform relaxation algorithm. The constants C_p and C_q depend on the problem parameters and the spatial dimension $N \geq 2$ of the problem (3.1), as shown in Table 2. In the table, ζ represents the smallest positive root of the polynomial

$$P(\zeta) = 3\pi^2\nu^2(8\nu-1)\zeta^3 - 4\pi^4(1-4\nu-100\nu^2+320\nu^3)\zeta^2 + 128\pi^6(48\nu^3+3-12\nu-10\nu^2)\zeta - 1024\pi^8(2\nu-1)^2,$$

$w = \sqrt{\pi^2\nu^2(N-1)^2+1}$, $\bar{\nu}_2$ is the root of the equation

$$\nu = \frac{1}{2}((a^2+4\nu b)(N-1))^{\frac{1}{4}} - \frac{1}{8}((a^2+4\nu b)(N-1))^{\frac{1}{2}},$$

which leads to the constants

$$\bar{\nu}_1 = \sqrt{N-1}\frac{b\sqrt{N-1}+\sqrt{b^2(N-1)+16a^2}}{32},$$

$$\bar{\nu}_2 \sim \frac{a^2\sqrt{a\sqrt{N-1}}(4-\sqrt{a\sqrt{N-1}})}{2(4a^2-2b\sqrt{a\sqrt{N-1}}+ab\sqrt{N-1})},$$

$$\bar{\nu}_3 = \frac{1}{32}\pi(N-1),$$

$$\bar{\nu}_4 = \frac{\pi(N-1)\left(\pi^5(N-1)^5+80\pi^3(N-1)^3+512\pi(N-1)+\sqrt{(3\pi^2(N-1)^2+16)(\pi^2(N-1)^2+16)^4}\right)}{16(\pi^6(N-1)^6+56\pi^4(N-1)^4+640\pi^2(N-1)^2+2048)},$$

$$\bar{\nu}_5 = \frac{4096-2048\pi(N-1)+256\pi^2(N-1)^2+128\pi^3(N-1)^3-16\pi^4(N-1)^4-\pi^6(N-1)^6+\sqrt{d}}{1024\pi^3(N-1)^3},$$

$$d = (\pi(N-1)-4)(\pi^3(N-1)^3+4\pi^2(N-1)^2+48\pi(N-1)-64)(\pi^2(N-1)^2+16)^4.$$

Finally, $\bar{\nu}_6 = \bar{\nu}_6(N)$ is defined by equalizing the constant C_p (or C_q) of the first two cases of $\beta = 2$ in Table 2, and is shown graphically, together with the other constants, in Figure 4.

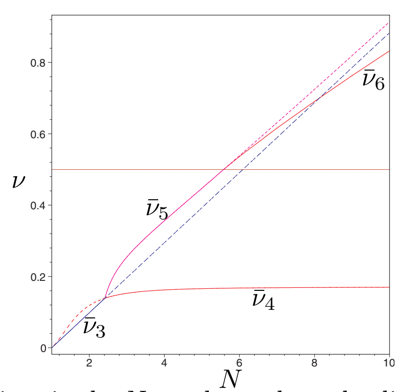

FIGURE 4. Regions in the $N-\nu$ plane where the different constants C_p and C_q of the optimized parameters in dimension $N \geq 2$ apply according to Table 2.

In the case with overlap, the optimal parameters in the transmission conditions are asymptotically given by $p = C_p\Delta x^{-\frac{1}{5}}$ and $q = C_q\Delta x^{\frac{3}{5}}$, where the constants C_p and C_q depend on the problem parameters, as shown in Table 3. The optimized convergence factor of the associated algorithm with this choice is given by $1 - O(\Delta x^{\frac{1}{5}})$. It is interesting to note that in the case with overlap, the results are independent of the dimension for $N \geq 2$.

Table 2. Summary of the constants in the asymptotically optimized parameters $p = C_p \Delta x^{-\frac{1}{4}}$ and $q = C_q \Delta x^{\frac{3}{4}}$ in dimension $N \geq 2$ in the nonoverlapping case, for $\Delta t = \Delta x^{\beta}$, $\beta = 1, 2$. The constants $\bar{\nu}_1$ up to $\bar{\nu}_6$, ζ and w are defined in the text.

β	ν	C_p and C_q
1	$\begin{cases} \bar{\nu}_1 \leq \frac{1}{2} \text{ and } \nu > \frac{1}{2} \\ \bar{\nu}_1 > \frac{1}{2} \text{ and } \nu > \bar{\nu}_2 \end{cases}$	$\begin{cases} C_p = \left(\frac{\nu\pi(a^2+4\nu b)^{\frac{3}{2}}\sqrt{N-1}}{2}\right)^{\frac{1}{4}} \\ C_q = \left(\frac{8\nu}{\pi^3(N-1)^{\frac{3}{2}}\sqrt{a^2+4\nu b}}\right)^{\frac{1}{4}} \end{cases}$
	$\bar{\nu}_1 < \nu \leq \frac{1}{2}$	$\begin{cases} C_p = \left(\frac{\pi\sqrt{(a^2+4\nu b)^3(N-1)}}{4}\right)^{\frac{1}{4}} \\ C_q = \left(\frac{4}{\pi^3\sqrt{(a^2+4\nu b)(N-1)^3}}\right)^{\frac{1}{4}} \end{cases}$
	$\begin{cases} \bar{\nu}_1 \leq \frac{1}{2} \text{ and } \nu \leq \bar{\nu}_1 \\ \bar{\nu}_1 > \frac{1}{2} \text{ and } \nu \leq \bar{\nu}_2 \end{cases}$	$\begin{cases} C_p = \left(\frac{8\nu\pi(a^2+4\nu b)^2(N-1)}{(8\nu+\sqrt{(a^2+4\nu b)(N-1)})^2}\right)^{\frac{1}{4}} \\ C_q = \left(\frac{128\nu}{\pi^3(N-1)(8\nu+\sqrt{(a^2+4\nu b)(N-1)})^2}\right)^{\frac{1}{4}} \end{cases}$
2	$\begin{cases} \nu > \frac{1}{2} \text{ and } N \leq 5 \\ \nu > \bar{\nu}_6 \text{ and } N \geq 6 \end{cases}$	$\begin{cases} C_p = \left(\frac{\nu^3(a^2+4\nu b)^3(\zeta^4+16\pi^2)^2}{2(\sqrt{\nu^2\zeta^4+\pi^2}+\nu\zeta^2)(\zeta^2+4\sqrt{\nu^2\zeta^4+\pi^2}-4\nu\zeta^2)^2}\right)^{\frac{1}{8}} \\ C_q = \left(\frac{8(\sqrt{\nu^2\zeta^4+\pi^2}+\nu\zeta^2)^3(\zeta^2+4\sqrt{\nu^2\zeta^4+\pi^2}-4\nu\zeta^2)^6}{\nu(a^2+4\nu b)(\zeta^4+16\pi^2)^6}\right)^{\frac{1}{8}} \end{cases}$
	$\frac{1}{2} < \nu \leq \bar{\nu}_6$ and $N \geq 6$	$\begin{cases} C_p = \left(\frac{\pi\nu^3(a^2+4\nu b)^3(\pi^2(N-1)^2+16)^2}{2(\pi(N-1)(1-4\nu)+4w)^2(\nu\pi(N-1)+w)}\right)^{\frac{1}{8}} \\ C_q = \left(\frac{8(\pi(N-1)(1-4\nu)+4w)^6(\nu\pi(N-1)+w)^3}{\pi^3\nu(a^2+4\nu b)(\pi^2(N-1)^2+16)^6}\right)^{\frac{1}{8}} \end{cases}$
	$\bar{\nu}_5 < \nu \leq \frac{1}{2}$ and $2 \leq N \leq 5$	$\begin{cases} C_p = (2\nu\pi(a^2+4\nu b)^3)^{\frac{1}{8}} \\ C_q = \left(\frac{1}{2048(\nu\pi)^3(a^2+4\nu b)}\right)^{\frac{1}{8}} \end{cases}$
	$\begin{cases} \bar{\nu}_4 < \nu \leq \bar{\nu}_5 \text{ and } 2 \leq N \leq 5 \\ \bar{\nu}_4 < \nu \leq \frac{1}{2} \text{ and } N \geq 6 \end{cases}$	$\begin{cases} C_p = \left(\frac{\pi\nu(a^2+4\nu b)^3(\pi^2(N-1)^2+16)^2}{8(\pi(N-1)(1-4\nu)+4w)^2(\nu\pi(N-1)+w)}\right)^{\frac{1}{8}} \\ C_q = \left(\frac{2(\pi(N-1)(1-4\nu)+4w)^6(\nu\pi(N-1)+w)^3}{\pi^3\nu^3(a^2+4\nu b)(\pi^2(N-1)^2+16)^6}\right)^{\frac{1}{8}} \end{cases}$
	$\nu \leq \bar{\nu}_4$ and $N \geq 2$	$\begin{cases} C_p = \left(\frac{\pi\sqrt{(N-1)(a^2+4\nu b)^3}}{4}\right)^{\frac{1}{4}} \\ C_q = \left(\frac{4}{\pi^3\sqrt{(N-1)^3(a^2+4\nu b)}}\right)^{\frac{1}{4}} \end{cases}$

Table 3. Summary of the constants in the optimized asymptotic parameters $p = C_p \Delta x^{-\frac{1}{5}}$ and $q = C_q \Delta x^{\frac{3}{5}}$ for the case with overlap $L = \Delta x$ in dimension $N \geq 2$ for $\Delta t = \Delta x^{\beta}$.

β	ν	C_p	C_q
1	$\nu > \frac{1}{2}$	$(\frac{1}{4}\nu(a^2+4\nu b)^2)^{\frac{1}{5}}$	$\left(\frac{64\nu^2}{(a^2+4\nu b)}\right)^{\frac{1}{5}}$
1	$\nu \leq \frac{1}{2}$	$\left(\frac{(a^2+4\nu b)^2}{8}\right)^{\frac{1}{5}}$	$\left(\frac{16}{a^2+4\nu b}\right)^{\frac{1}{5}}$
2	$\nu > \frac{1}{2}$	$(2\nu^2(a^2+4\nu b)^2)^{\frac{1}{5}}$	$\left(\frac{1}{8\nu(a^2+4\nu b)}\right)^{\frac{1}{5}}$
2	$\frac{1}{8} < \nu \leq \frac{1}{2}$	$(\nu(a^2+4\nu b)^2)^{\frac{1}{5}}$	$\left(\frac{1}{32\nu^3(a^2+4\nu b)}\right)^{\frac{1}{5}}$
2	$\nu \leq \frac{1}{8}$	$\left(\frac{(a^2+4\nu b)^2}{8}\right)^{\frac{1}{5}}$	$\left(\frac{16}{a^2+4\nu b}\right)^{\frac{1}{5}}$

5. Well-posedness and convergence of the Schwarz waveform relaxation algorithms

For the analysis in this section, we rely on the theory of weak solution in Sobolev spaces by a Galerkin method; see [2] and [29]. A weak solution of (3.1) is defined to be a $u \in \mathcal{C}(0,T;L^2(\Omega)) \cap L^2(0,T;H^1(\Omega))$, such that, for any v in $H^1(\Omega)$, we have

$$\frac{d}{dt}(u,v)+\frac{1}{2}\big(((\boldsymbol{a}\cdot\boldsymbol{\nabla})u,v)-((\boldsymbol{a}\cdot\boldsymbol{\nabla})v,u)\big)+\nu(\nabla u,\nabla v)+b(u,v)=(f,v), \text{ in } \mathcal{D}'(0,T), \tag{5.1}$$

where $(\cdot,\cdot)$ denotes the inner product in $L^2(\Omega)$. Problem (5.1) is completed by the initial condition

$$u(x,0) = u_0(x), \quad \text{in } \Omega. \tag{5.2}$$

The next two theorems show the well-posedness and the regularity of the problem.

Theorem 5.1 (Existence and uniqueness)**.** *Let $\Omega = \mathbb{R}^N$. If the initial value u_0 is in $L^2(\Omega)$, and the right-hand side f is in $L^2(0,T;L^2(\Omega))$, then there exists a unique weak solution u of* (5.1), (5.2) *in $L^\infty(0,T;L^2(\Omega)) \cap L^2(0,T;H^1(\Omega))$.*

With the transmission conditions given by $\mathcal{B}_j$ in (3.11), we will need more regularity in our analysis, in the anisotropic Sobolev spaces defined in [29] by

$$H^{r,s}(\Omega \times (0,T)) = L^2(0,T;H^r(\Omega)) \cap H^s(0,T;L^2(\Omega)).$$

Theorem 5.2. *Let $\Omega = \mathbb{R}^N$, and m be an integer. If the initial value u_0 is in $H^{2m+1}(\Omega)$, and the right-hand side f is in $H^{2m,m}(\Omega \times (0,T))$, then the weak solution u is in $H^{2(m+1),m+1}(\Omega \times (0,T))$.*

For the proofs of Theorems 5.1 and 5.2, and the trace theorems in $H^{r,s}$, we refer to [29].

5.1. **Well-posedness of the algorithm.** We first need to study the well-posedness of the subdomain problems with the new boundary conditions. As we saw in the previous section, in order for the convergence factor to be smaller than 1 in modulus, we need $p > 0, q \geq 0$. The special case where $q = 0$ can be found in [31], and hence, in the sequel, we assume $q \neq 0$. We show here only the analysis for the subproblem on Ω_1, the results for Ω_2 can be found similarly by symmetry.

The boundary of Ω_1 is $\Gamma_L = \{L\} \times \mathbb{R}^{N-1}$. Using the boundary operators $\mathcal{S}$ and $\mathcal{B}_1$ defined in (3.11), the problem consists of finding v in an adapted subspace of $\mathcal{C}(0,T;L^2(\Omega_1)) \cap L^2(0,T;H^1(\Omega_1))$ such that

$$\begin{array}{rcll} \mathcal{L}v &=& f & \text{in } \Omega_1 \times (0,T), \\ v(\cdot,0) &=& u_0 & \text{in } \Omega_1, \\ \mathcal{B}_1 v &=& g_L & \text{on } \Gamma_L \times (0,T). \end{array} \tag{5.3}$$

For the variational formulation, we introduce for any real number s the space

$$H^s_s(\Omega_1) = \{v \in H^s(\Omega_1), v_{|\Gamma_L} \in H^s(\Gamma_L)\},$$

where $\cdot_{|\Gamma_L}$ denotes the trace operator on Γ_L. The scalar product in $L^2(\Gamma_L)$ is denoted by $(\cdot,\cdot)_{\Gamma_L}$. The variational formulation is to find $v \in H^1_1$ such that,

$$\begin{aligned} &\forall w \in H^1_1(\Omega_1), \frac{d}{dt}\big[(v,w) + 2q(v,w)_{\Gamma_L}\big] \\ &\quad + \frac{1}{2}\big(((\boldsymbol{a}\cdot\boldsymbol{\nabla})v,w) - ((\boldsymbol{a}\cdot\boldsymbol{\nabla})v,w)\big) + \nu(\boldsymbol{\nabla}v,\boldsymbol{\nabla}w) + b(v,w) \\ &\quad + \frac{p}{2}(v,w)_{\Gamma_L} + 2q\nu((\boldsymbol{c}\cdot\boldsymbol{\nabla_y})v,w)_{\Gamma_L} + 2q\nu^2(\boldsymbol{\nabla_y}v,\boldsymbol{\nabla_y}w)_{\Gamma_L} = (f,v), \text{ in } \mathcal{D}'(0,T). \end{aligned}$$

Theorem 5.3. *For $p > 0$ and $q > 0$, if f is in $L^2(0,T,L^2(\Omega_1))$, u_0 is in $H^1_1(\Omega_1)$, and g_L is in $L^2((0,T)\times\Gamma_L)$, then the subdomain problem* (5.3) *has a unique solution v in $L^2(0,T,H^2_2(\Omega_1)) \cap H^1(0,T;H^0_0(\Omega_1))$.*

Proof. The proof is based on *a priori* estimates: multiplying equation (5.3) by v and integrating in space, and then using the boundary condition, we obtain

$$\begin{aligned} &\frac{1}{2}\frac{d}{dt}\left[\|v(\cdot,t)\|^2_{L^2(\Omega_1)} + 2q\|v(\cdot,t)\|^2_{L^2(\Gamma_L)}\right] + \nu\|\boldsymbol{\nabla}v(\cdot,t)\|^2_{L^2(\Omega_1)} + b\|v(\cdot,t)\|^2_{L^2(\Omega_1)} \\ &+ \frac{p}{2}\|v(\cdot,t)\|^2_{L^2(\Gamma_L)} + 2q\nu^2\|\boldsymbol{\nabla_y}v(\cdot,t)\|^2_{L^2(\Gamma_L)} = (f(\cdot,t),v(\cdot,t)) + \nu(g(\cdot,t),v(\cdot,t))_{\Gamma_L}. \end{aligned}$$

On the right-hand side we use the Cauchy-Schwarz inequality together with the inequality

$$\alpha\beta \le \frac{\eta}{2}\,\alpha^2 + \frac{1}{2\eta}\,\beta^2, \quad \text{for all } \alpha,\beta \in \mathbb{R}, \text{ and } \eta > 0. \tag{5.4}$$

If $b = 0$, we need in addition the Gronwall Lemma. We obtain by integration in time a bound for v, with a constant C depending on the physical constants b, ν, the parameters p and q, and the length of the time interval T:

$$\begin{aligned} &\|v\|^2_{L^\infty(0,T,H^0_0(\Omega_1))} + \|v\|^2_{L^2(0,T;H^1_1(\Omega_1))} \\ &\qquad \le C(\|f\|^2_{L^2(0,T,L^2(\Omega_1))} + \|g\|^2_{L^2(0,T,L^2(\Gamma_L))}). \end{aligned} \tag{5.5}$$

To get further estimates, we multiply equation (5.3) by $\partial_t v$, integrate in space, and use the boundary condition to obtain

$$\begin{aligned} &\tfrac{1}{2}\tfrac{d}{dt}\left[b\|v(\cdot,t)\|^2_{L^2(\Omega_1)} + \nu\|\boldsymbol{\nabla}v(\cdot,t)\|^2_{L^2(\Omega_1)} + \tfrac{p-a}{2}\|v(\cdot,t)\|^2_{L^2(\Gamma_L)} + q\nu^2\|\boldsymbol{\nabla_y}v(\cdot,t)\|^2_{L^2(\Gamma)}\right] \\ &\quad + \|\partial_t v(\cdot,t)\|^2_{L^2(\Omega_1)} + 2q\|\partial_t v(\cdot,t)\|^2_{L^2(\Gamma_L)} = (f(\cdot,t),\partial_t v(\cdot,t)) + (g(\cdot,t),\partial_t v(\cdot,t))_{\Gamma_L} \\ &\qquad - ((\boldsymbol{a}\cdot\boldsymbol{\nabla})v(\cdot,t),\partial_t v(\cdot,t)) + 2q\nu((\boldsymbol{c}\cdot\boldsymbol{\nabla_y})v(\cdot,t),\partial_t v(\cdot,t))_{\Gamma_L}. \end{aligned}$$

Using the Cauchy-Schwarz inequality together with (5.4) as before, integrating in time and using (5.5), we obtain

$$\|v\|^2_{L^\infty(0,T,H^1_1(\Omega_1))} + \|\partial_t v\|^2_{L^2(0,T;H^0_0(\Omega_1))} \le C'(\|f\|^2_{L^2(0,T,L^2(\Omega_1))} + \|g\|^2_{L^2(0,T,L^2(\Gamma_L))}),$$

where the constant C' depends also on $\boldsymbol{a}$. We complete the result by using equation (5.3), which gives

$$\Delta v \in L^2(0,T;L^2(\Omega_1)), \quad \partial_x v - 2q\nu\Delta_{\boldsymbol{y}} v \in L^2(0,T;L^2(\Gamma_L)).$$

A regularity theorem proved in [39] asserts that this implies $v \in L^2(0,T;H^2_2(\Omega_1))$, and gives a bound for the norm in $L^2(0,T;H^2_2(\Omega_1))$. Now we have altogether a bound for v in $L^2(0,T,H^2_2) \cap H^1(0,T;H^0_0(\Omega_1))$. This first proves uniqueness. Using a Galerkin method, we obtain the existence result. □

The previous result suffices to define the algorithm in the nonoverlapping case. The overlapping case however requires more regularity.

Theorem 5.4. *For $p > 0$ and $q > 0$, let f be in $H^{2,1}(\Omega_1 \times (0,T))$, u_0 be in $H^3(\Omega)$, and g_L be in $H^{\frac{3}{2},\frac{3}{4}}(\Gamma_L \times (0,T))$, with the compatibility condition*

$$\begin{aligned} g_L(\cdot,0) = \partial_x u_0(L,\cdot) &+ \frac{p-a}{2\nu} u_0(L,\cdot) \\ &+ 2q(\nu\partial_{xx}u_0(L,\cdot) - a\partial_x u_0(L,\cdot) - bu_0(L,\cdot) + f(L,\cdot,0)). \end{aligned} \tag{5.6}$$

Then the solution v of the subdomain problem (5.3) is in $H^{4,2}(\Omega_1 \times (0,T))$. Furthermore, the following compatibility property at $x = 0$ is satisfied:

$$\begin{aligned} \lim_{t\to 0+} \mathcal{B}_2 v(0,\cdot,t) = \partial_x u_0(0,\cdot) &- \frac{p+a}{2\nu} u_0(0,\cdot) \\ &- 2q(\nu\partial_{xx}u_0(0,\cdot) - a\partial_x u_0(0,\cdot) - bu_0(0,\cdot) + f(0,\cdot,0)). \end{aligned}$$

Proof. With the assumptions in the theorem, the solution u of (3.1) is indeed in $H^{4,2}(\Omega_1 \times (0,T))$ by Theorem 5.2, and by the Trace Theorem in [29], $\tilde{g}_L = \mathcal{B}_1 u(L,\cdot,\cdot)$ is in $H^{\frac{3}{2},\frac{3}{4}}(\Gamma_L \times (0,T))$, and satisfies the compatibility condition (5.6). Defining $h = g_L - \tilde{g}_L$, $e = v - u$ is the solution of

$$\begin{aligned} \mathcal{L}e &= 0 \quad \text{in } \Omega_1 \times (0,T), \\ e(\cdot,0) &= 0 \quad \text{in } \Omega_1, \\ \mathcal{B}_1 e &= h \quad \text{on } \Gamma_L \times (0,T). \end{aligned} \tag{5.7}$$

Since h is in $H^{\frac{3}{2},\frac{3}{4}}(\Gamma_L \times (0,T))$, and $h(\cdot,0) = 0$, we can extend it in $H^{\frac{3}{2},\frac{3}{4}}(\Gamma_L \times \mathbb{R})$ by $\tilde{h}$ vanishing on $\Gamma \times \mathbb{R}_-$. Then we extend in time the first equation and the boundary condition in (5.7) to $\Gamma_L \times \mathbb{R}$. The solution $\tilde{e}$ of the extended problem is an extension of e. We finally Fourier transform the resulting equation in time and $\boldsymbol{y}$. By (3.4), the Fourier transform of e is given in terms of $\mathcal{F}\tilde{h}$, the Fourier transform of $\tilde{h}$, by

$$\mathcal{F}\tilde{e}(\boldsymbol{\eta},\omega) = \frac{2\nu}{f(z)+s(z)} \mathcal{F}\tilde{h}(\boldsymbol{\eta},\omega) e^{\frac{a+f(z)}{2\nu}(x-L)}, \tag{5.8}$$

with $z = i(\omega + \boldsymbol{c}\cdot\boldsymbol{\eta}) + \nu|\boldsymbol{\eta}|^2$. We introduce $\tau = \omega + \boldsymbol{c}\cdot\boldsymbol{\eta}$. With the definition of f, and using that $p > 0$, $q > 0$, we obtain

Lemma 5.5. *There exist positive constants D, D' such that*

$$\begin{aligned} \frac{2\nu}{|f(z)+s(z)|} &\le D(\tau^2 + |\boldsymbol{\eta}|^4)^{-1/2}, \\ \frac{\nu}{a + \Re f(z)} &\le D'(\tau^2 + |\boldsymbol{\eta}|^4)^{-1/4}, \end{aligned}$$

For large τ and $\boldsymbol{\eta}$, we have

$$|r^+|^2 \sim 2(\tau^2 + |\boldsymbol{\eta}|^4)^{1/2}.$$

From (5.8), for the norm of the second derivative of e in time, we obtain

$$\|\partial_t^2 \tilde{e}\|^2_{L^2(\Omega_1\times\mathbb{R})} = \int_{-\infty}^{L}\int_{\mathbb{R}^{n-1}}\int_{\mathbb{R}} \frac{4\nu^2\omega^4}{\big|f(z)+s(z)\big|^2}\ |\mathcal{F}\tilde{h}(\boldsymbol{\eta},\omega)|^2 e^{2\Re r^+(x-L)}dx\, d\boldsymbol{\eta}\, d\omega,$$

or after integration in the x variable,

$$\|\partial_t^2 \tilde{e}\|^2_{L^2(\Omega_1\times\mathbb{R})} = \int_{\mathbb{R}^{n-1}}\int_{\mathbb{R}} \frac{4\nu^2\omega^4}{\big|f(z)+s(z)\big|^2}\ \frac{\nu}{a+\Re f(z)}|\mathcal{F}\tilde{h}(\boldsymbol{\eta},\omega)|^2 d\boldsymbol{\eta}\, d\omega.$$

We have by Lemma 5.5, for large τ and $\boldsymbol{\eta}$,

$$\begin{aligned}\tfrac{4\nu^2\omega^4}{\big|f(z)+s(z)\big|^2}\ \tfrac{\nu}{a+\Re f(z)} &\le D^2D'(\tau - \boldsymbol{c}\cdot\boldsymbol{\eta})^4(\tau^2+|\boldsymbol{\eta}|^4)^{5/4}\\ &= D^2D'\tfrac{(\tau-\boldsymbol{c}\cdot\boldsymbol{\eta})^4}{(\tau^2+|\boldsymbol{\eta}|^4)^2}(\tau^2+|\boldsymbol{\eta}|^4)^{3/4}.\end{aligned}$$

Since $\tilde{h}$ is in $H^{\frac{3}{2},\frac{3}{4}}(\Gamma_L\times\mathbb{R})$, we obtain

$$\|\partial_t^2 \tilde{e}\|^2_{L^2(\Omega_1\times\mathbb{R}^2)} \le D''\|\tilde{h}\|^2_{H^{\frac{3}{2},\frac{3}{4}}(\Gamma_L\times\mathbb{R})}.$$

For the spatial derivatives, we proceed as before, and we have for $j+k\le 4$,

$$\|\partial_x^k\partial_{y_l}^j \tilde{e}\|^2_{L^2(\Omega_1\times\mathbb{R})} = \int_{\mathbb{R}^{n-1}\times\mathbb{R}} \frac{4\nu^2 r_+^{2k}\eta_l^{2j}}{\big|f(z)+s(z)\big|^2}\ \frac{\nu}{a+\Re f(z)}|\mathcal{F}\tilde{h}(\omega)|^2 d\boldsymbol{\eta}\, d\omega.$$

From the bound on the integrand for large τ and $\boldsymbol{\eta}$,

$$\frac{4\nu^2 r_+^{2k}\eta_l^{2j}}{\big|f(z)+s(z)\big|^2}\ \frac{\nu}{a+\Re f(z)} \le D^2D'2^k(\tau^2+|\boldsymbol{\eta}|^4)^{(k+j)/2},$$

we conclude as before that all space derivatives up to order 4 are square integrable, and finally we have

$$\|\tilde{e}\|_{H^{4,2}(\Omega_1\times\mathbb{R})} \le \bar{D}\|\tilde{h}\|_{H^{\frac{3}{2},\frac{3}{4}}(\Gamma_L\times\mathbb{R})}.$$

Taking the infimum over all extensions $\tilde{h}$ gives

$$\|e\|_{H^{4,2}(\Omega_1\times(0,T))} \le C\|h\|_{H^{\frac{3}{2},\frac{3}{4}}(\Gamma_L\times(0,T))}.$$

Similarly, we see that

$$\begin{aligned}&\|\mathcal{S}\tilde{e}(0,\cdot,\cdot)\|^2_{H^{\frac{3}{2},\frac{3}{4}}(\Gamma_L\times\mathbb{R})}\\ &\quad= \int_{\mathbb{R}^{n-1}\times\mathbb{R}} \frac{4\nu^2|z|^2(1+\omega^2)^{\frac{3}{2}}(1+|\boldsymbol{\eta}|^2)^3}{\big|f(z)+s(z)\big|^2}e^{-2\Re r^+L}\,|\mathcal{F}\tilde{h}(\omega)|^2 d\boldsymbol{\eta}\, d\omega\,,\end{aligned}$$

and therefore $\mathcal{S}e(0,\cdot)$ is in $H^{\frac{3}{2},\frac{3}{4}}(\Gamma_L\times(0,T))$, with

$$\|\mathcal{S}e\|^2_{H^{\frac{3}{2},\frac{3}{4}}(\Gamma_L\times(0,T))} \le Ce^{-\frac{aL}{\nu}}\|h\|_{H^{\frac{3}{2},\frac{3}{4}}(\Gamma_L\times(0,T))}.$$

For the compatibility property, since $\tilde{h}$ is supported in $\Gamma_L\times\mathbb{R}_+$, $\mathcal{F}\tilde{h}$ is analytic in the half-plane $\Im\omega<0$, and by (5.8) and the Paley-Wiener Theorem [36], $\tilde{e}(0,\cdot,\cdot)$ is supported in $\Gamma_L\times\mathbb{R}_+$ as well. Since e is in $H^{4,2}(\Omega_1\times(0,T))$, $\partial_x e$ is in $H^{\frac{5}{2},\frac{5}{4}}(\Gamma_L\times(0,T))$, and hence all quantities in $\mathcal{B}_2 e$ are continuous on $[0,T]$, and therefore $\lim_{t\to 0_+}\mathcal{B}_2 e(0,\cdot,t)=0$, which completes the proof of the theorem. ☐

We are now ready to show the well-posedness of the algorithm: let g_L be given on Γ_L and let g_0 be given on $\Gamma_0 = \{0\} \times \mathbb{R}^{N-1}$, and let $p > 0$ and $q > 0$. We define for $k = 1, 2, \ldots$ the iterations by algorithm (3.2), initialized by

$$\mathcal{B}_1 u_1^1 = g_L \text{ on } \Gamma_L \times (0,T), \quad \mathcal{B}_2 u_2^1 = g_0 \text{ on } \Gamma_0 \times (0,T). \tag{5.9}$$

Consider first the nonoverlapping case: $L = 0$. Then it is easy to obtain:

Theorem 5.6. *Let $L = 0$, g_L and g_0 be given in $L^2(\mathbb{R}^{n-1} \times (0,T))$, $p > 0$ and $q > 0$. Then, for $k = 1, 2, \ldots$, the algorithm* (3.2) *with the transmission operators given in* (3.11)*, initialized with* (5.9) *defines a unique sequence of iterates (u_1^k, u_2^k) in $L^2(0,T,H_2^2(\Omega_1)) \cap H^1(0,T;H_0^0(\Omega_1)) \times L^2(0,T,H_2^2(\Omega_2)) \cap H^1(0,T;H_0^0(\Omega_2))$.*

In the overlapping case, we need to use the compatibility condition in Theorem 5.4:

Theorem 5.7. *Let $L > 0$, $p > 0$ and $q > 0$, let f be in $H^{2,1}(\Omega_1 \times (0,T))$, u_0 in $H^3(\Omega)$, and let g_0 and g_L be given in $H^{\frac{3}{2},\frac{3}{4}}(\mathbb{R}^{n-1} \times (0,T))$, with the compatibility conditions*

$$\begin{aligned} g_L(\cdot,0) &= \partial_x u_0(L,\cdot) + \frac{p-a}{2\nu} u_0(L,\cdot) \\ &\quad + 2q(\nu \partial_{xx} u_0(L,\cdot) - a\partial_x u_0(L,\cdot) - bu_0(L,\cdot) + f(L,\cdot,0)), \\ g_0(\cdot,0) &= \partial_x u_0(0,\cdot) - \frac{p+a}{2\nu} u_0(0,\cdot) \\ &\quad - 2q(\nu \partial_{xx} u_0(0,\cdot) - a\partial_x u_0(0,\cdot) - bu_0(0,\cdot) + f(0,\cdot,0)). \end{aligned}$$

Then, for $k = 1, 2, \ldots$, the algorithm (3.2) *with the transmission operators given in* (3.11)*, initialized by* (5.9) *defines a unique sequence of iterates (u_1^k, u_2^k) in $H^{4,2}(\Omega_1 \times (0,T)) \times H^{4,2}(\Omega_2 \times (0,T))$.*

5.2. **Convergence of the algorithm.**

Theorem 5.8. *For $p > 0$ and $q > 0$, under the conditions of existence of the algorithm, the sequence (u_1^k, u_2^k) converges to $(u_{|\Omega_1}, u_{|\Omega_2})$.*

Proof. We return to the analysis in Section 3, which has been validated by the previous theorems. The Fourier transforms in time and $\boldsymbol{y}$ of the errors satisfy

$$\begin{aligned} \hat{e}_1^{2k+1}(x,\boldsymbol{\eta},\omega) &= \rho^k \hat{e}_1^1(x,\boldsymbol{\eta},\omega), \quad \hat{e}_1^{2k}(x,\boldsymbol{\eta},\omega) = \rho^{k-1} \hat{e}_2^1(x,\boldsymbol{\eta},\omega), \\ \hat{e}_2^{2k+1}(x,\boldsymbol{\eta},\omega) &= \rho^k \hat{e}_2^1(x,\boldsymbol{\eta},\omega), \quad \hat{e}_2^{2k}(x,\boldsymbol{\eta},\omega) = \rho^{k-1} \hat{e}_1^1(x,\boldsymbol{\eta},\omega). \end{aligned}$$

For p and q strictly positive, we have $|\rho| < 1$ for all $(\omega, \boldsymbol{\eta})$ in $(\mathbb{R} \times \mathbb{R}^{n-1})$. By the Lebesgue Theorem, we conclude the proof. □

Remark 5.9. The results in this section generalize the analysis from [31] to the case when the operator S contains the transverse Laplace operator Δ_y. In [31], however, the proof of convergence in the nonoverlapping case is based on clever energy estimates, and extends to variable coefficients.

6. Numerical results

We perform in this section one-dimensional numerical experiments to measure the convergence factors of the numerical implementation of the various Schwarz waveform relaxation algorithms analyzed at the continuous level in this paper. We use the parabolic model problem (3.1) on the domain $\Omega = (0, 6)$. We impose homogeneous boundary conditions, $u(0,t) = 0$ and $u(6,t) = 0$, and use various initial conditions $u(x,0)$, $x \in \Omega$.

6.1. **Experiments with two subdomains.** We first use a decomposition of the domain Ω into the two subdomains $\Omega_1 = (0, L_2)$ and $\Omega_2 = (L_1, 6)$, $L_1 \le L_2$, and hence $L = L_2 - L_1$. We denote by one iteration here a double iteration of the respective algorithms, since for two subdomains, one can perform all the iterations in an alternating fashion and thus obtain the even iterates on one subdomain and the odd ones on the other, without having to compute the remaining ones. We show only results of numerical experiments for the algorithm with overlap, since with overlap, we can compare the results to the classical Schwarz waveform relaxation algorithm with Dirichlet transmission conditions, which does not converge without overlap. We choose for the problem parameters $\nu = 0.2$, $a = 1$, $b = 0$. We discretize (3.1) using an upwind finite difference discretization in space with mesh parameter $\Delta x = 0.02$, and a backward Euler discretization in time, with time step $\Delta t = 0.005$. We choose $L_1 = 2.96$ and $L_2 = 3.04$, which means the overlap is $L = 0.08$, and we compute the numerical solution in the time interval $[0, T = 2.5]$. Using as initial condition

$$u(x,0) = e^{-3(1.2-x)^2},$$

we have already shown in Figure 3 for this example the first few iterations at the end of the time interval $T = 2.5$, where we started the algorithm with a zero initial guess, both for the classical and the optimized waveform relaxation algorithm. In Figure 5 on the left, one can see how the error decreases as the iteration progresses for the classical algorithm, the one with first order Taylor conditions, $p = p_T = 1$ and $q = q_T = 0.4$, and with optimized parameters, which were found to be $p = p^* = 1.366061845$ and $q = q^* = 0.1363805228$ using Theorem 4.12. By error we denote here the discrete L^2 norm in time of the difference between the converged solution and the current iteration at the interface of Ω_1. It is important to realize that the computational cost per iteration of all these algorithms is the same: a change in the transmission conditions does not affect the local solver cost on each subdomain.

In Figure 5 on the right, we performed five iterations of the optimized Schwarz waveform relaxation algorithm with first order transmission conditions, varying the free parameters p and q, and show the base 10 logarithm of the error obtained. We indicate by a star the optimal parameters p^*, q^* predicted by Theorem 4.12. This shows that the continuous analysis predicts the optimal choice very well.

To illustrate the asymptotic results given in Theorem 4.4 for the Taylor conditions and in Theorem 4.14 for the optimized ones, we choose the same problem parameters as before, but start now with a coarser mesh both in space and time, $\Delta x = 0.04$ and $\Delta t = 0.01$, and we fix the overlap to be $L = \Delta x$. We then run the optimized Schwarz waveform relaxation algorithm with first order Taylor and optimized transmission conditions until the error becomes smaller than 10^{-14}, and count the number of iterations. We repeat this experiment dividing Δx and Δt by 2 several times. This corresponds for the first order Taylor conditions to the case in Theorem 4.4 where the convergence factor should behave like $1 - O(\sqrt{\Delta x})$, and for the first order optimized conditions to the case in Theorem 4.14 where the conver-

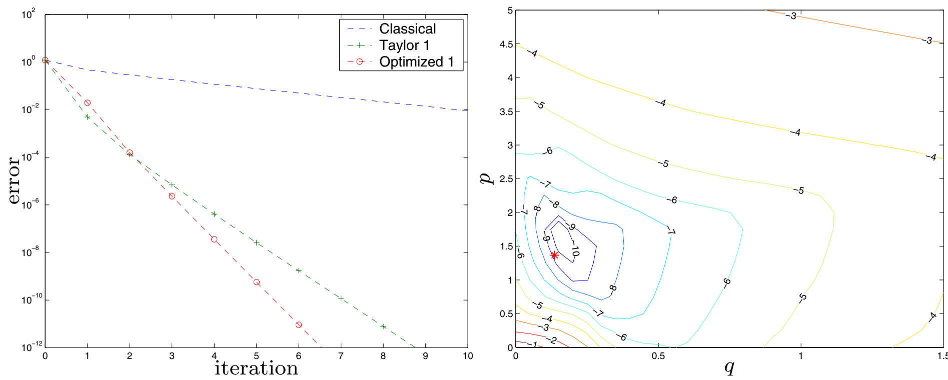

FIGURE 5. Left: convergence curves of the classical Schwarz waveform relaxation algorithm with Dirichlet transmission conditions compared to the same algorithm with the new first order transmission conditions. Right: the error obtained running the algorithm with first order transmission conditions for 5 steps and various choices of the free parameters p and q, and indicated by a star the choice p^*, q^* predicted by the theory.

gence factor should behave like $1 - O(\Delta x^{\frac{1}{8}})$, almost independent of Δx. Figure 6 shows on the left the results obtained from these experiments. One can see that the asymptotic analysis predicts very well the numerical behavior of the algorithms. Next, we perform a similar experiment, starting with the same values for Δx and Δt, but now we divide Δx by 2 each time and Δt only by $\sqrt{2}$ (such a refinement is admissible, since our scheme is implicit), which implies $\Delta t = O(\sqrt{\Delta x})$. While this does not change anything for the classical algorithm, which still has the same bad convergence factor $1 - O(\Delta x)$, for the algorithm with Taylor first order transmission conditions now case 3 of Theorem 4.4 applies, and the algorithm should show the much better convergence factor $1 - O(\Delta x^{\frac{1}{4}})$. The optimized Algorithm has according to Theorem 4.14 now the even better convergence factor $1 - O(\Delta x^{\frac{1}{16}})$, virtually independent of Δx. In Figure 6 on the right, one can clearly see that this is the case. The algorithm has different asymptotic convergence factors with the same overlap, depending on the discretization in time, as predicted.

6.2. **Experiments with eight subdomains.** We now show experiments which indicate that the results we obtained for two subdomains are also relevant for many subdomains. Using the same model problem as before, we now decompose the domain into eight subdomains. In Figure 7, we show in the top row the first 3 iterations of the classical Schwarz waveform relaxation algorithm, and below the same iterations for the algorithm with optimized first order transmission conditions. This clearly shows how important the transmission conditions are in the many subdomain case. We show the corresponding convergence factors in Figure 8 on the left, and on the right we perform the same asymptotic experiments as in Figure 6 on the left, but now with eight subdomains, which indicates that the results of Theorems 4.4 and 4.14 also hold for more than two subdomains.

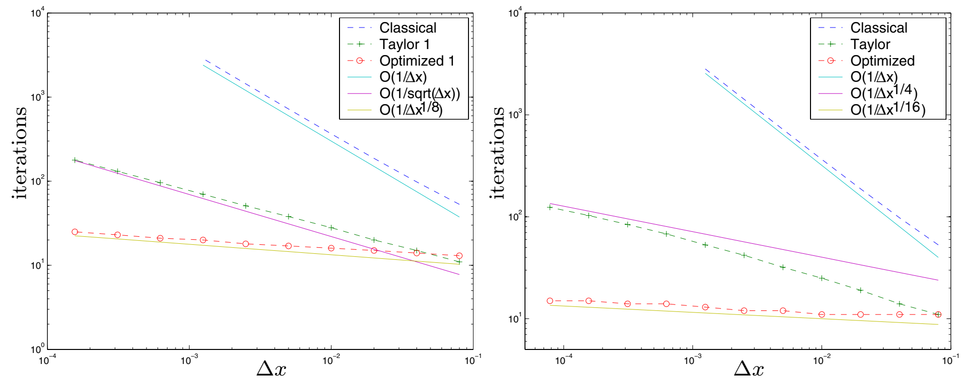

FIGURE 6. Asymptotic behavior as the mesh is refined with an overlap $L = \Delta x$: on the left the case where $\Delta t = O(\Delta x)$ and on the right where $\Delta t = O(\sqrt{\Delta x})$, together with the predicted rates from the analysis, both for the classical and the optimized Schwarz waveform relaxation algorithms with Taylor and optimized first order transmission conditions.

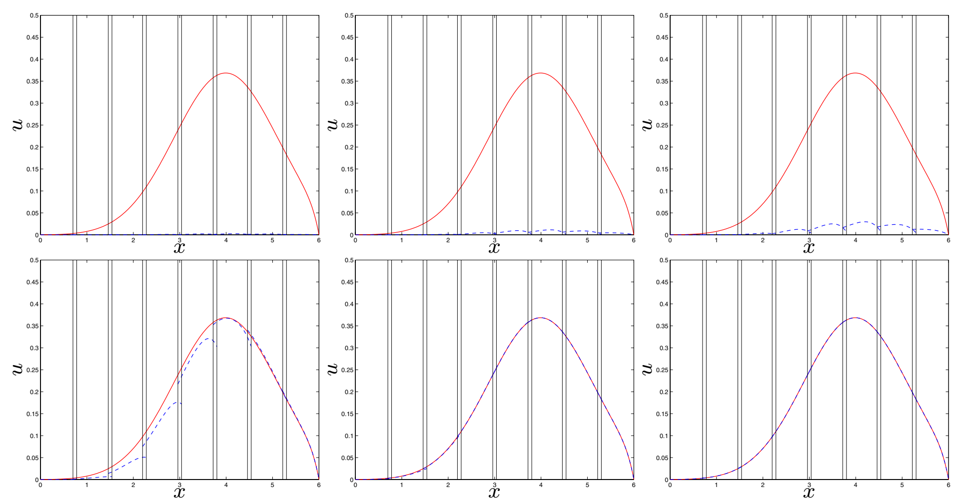

FIGURE 7. From left to right, the first, second and third iterates $u_j^k(x, T)$, $j = 1, \ldots, 8$ (dashed) at the end of the time interval $t = T$ together with the exact solution (solid) for the same model problem as before with eight subdomains: top row the classical and bottom row the optimized algorithm.

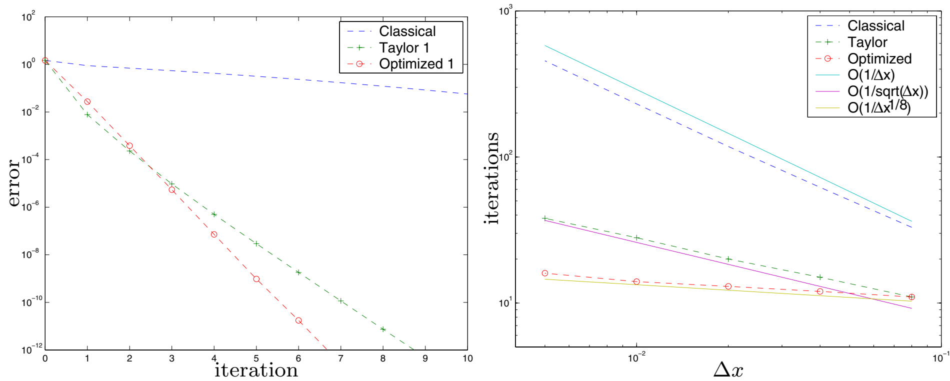

FIGURE 8. Left: convergence factor comparison for the eight subdomain case. Right: Asymptotic behavior as the mesh is refined with an overlap $L = \Delta x$ for the eight subdomain case, with $\Delta t = O(\Delta x)$, together with the predicted rates from the two subdomain analysis.

7. Conclusions

While zeroth order transmission conditions were optimized by direct analysis in [15] for an optimized Schwarz waveform relaxation algorithm applied to advection reaction diffusion problems, the solution of the homographic best approximation problem in this paper allowed us to find optimized first order transmission conditions, which lead to even better performance of the algorithm, at the same cost per iteration.

Similar homographic best approximation problems also occur in the design of optimized Schwarz methods for steady problems, and so far these problems have always been treated by direct analysis; see for example [26, 28, 27, 9] for advection diffusion problems, [7, 6, 19, 16] for indefinite Helmholtz problems, and [12] for the positive definite Helmholtz case. Our results here also apply to homographic best approximation problems from the steady case, and will thus be useful for the further development of optimized Schwarz methods; we currently study the application to indefinite Helmholtz problems.

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