# Neumann–Neumann Waveform Relaxation for the Time-Dependent Heat Equation

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### **1** Introduction

The goal of this paper is to introduce and analyze a new variant of waveform relaxation (WR) methods based on Neumann-Neumann iterations. Originally introduced by [13] for ODE systems, WR methods have first been used to solve time-dependent PDEs in [11] and [12]. When applying a WR method for a given domain  $\Omega$  and a decomposition into subdomains  $\{\Omega_i\}_{i=1}^N, \cup_i \overline{\Omega}_i = \overline{\Omega}$ , each iteration consists of solving independent subproblems on  $\Omega_i \times [0, T]$ , i.e., over the whole time window [0, T], before exchanging information across the interfaces; in other words, the information exchanged consists of interface traces over the time window [0, T]. This is in contrast with the classical approach, in which one fixes a time stepping strategy for the whole domain  $\Omega$  and uses domain decomposition to solve the resulting spatial problem at each time step. One advantage of the WR framework is that it allows the use of different spatial and time discretizations for each subdomain; this is especially useful for problems with large coefficient jumps [9] or with different models for different parts of the domain [8]. In addition, since communication between subdomains are less frequent than for the standard approach, there is a reduction in communication costs, particularly for networks with high latency.

Typically, WR methods can be derived from methods for elliptic PDEs. For example, one can extend the parallel Schwarz method with classical transmission conditions [14] to obtain the parallel Schwarz WR method; this has been analyzed in [11, 12]. WR extensions based on optimized Schwarz methods [6] have also been proposed. Substructuring methods form another class of methods for elliptic PDEs: examples include the Neumann–Neumann method [2, 4], as well as the FETI method [5] and its variants. However, to the best of our knowledge, no substructuring-type analogue of WR has been proposed, despite substructuring methods having many attractive properties for elliptic problems, such as mesh independence in the two-subdomain case. Thus, our first aim is to define the Neumann–Neumann waveform relaxation (NNWR) method, which generalizes the elliptic Neumann–Neumann method in a natural way. This is done in Section 2.

Our second goal is to understand the convergence of the proposed algorithm for parabolic problems. For systems of ODEs, a Picard–Lindelöf type argument shows that convergence is superlinear on bounded time intervals [0,T], with an error estimate of the form  $(CT)^k/k!$  after k iterations [16]. For overlapping Schwarz WR methods applied to the advection-diffusion equation, the estimate can be improved

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to  $e^{-(kL)^2/T}$ , where *L* is the size of the overlap [12]; this bound is possible because of the diffusivity of the problem. However, for unbounded time intervals, only linear convergence can be expected [11]. Similar conclusions hold for Schwarz WR with optimized transmission conditions, with or without overlap [15, 7, 1]. Using the 1D heat equation as the model problem, we show that the NNWR method also converges superlinearly for finite time intervals; this is done in Section 3, with some numerical experiments confirming the results in Section 4. We also derive a linear bound that is valid for unbounded time intervals. We have chosen to analyze the method in the continuous setting because it allows us to understand the asymptotic behaviour of the algorithm for very fine grids, without requiring explicit knowledge of how each subdomain problem is discretized. For ease of presentation, we prove our results for two subdomains in one spatial dimension; [10] contains further results, some of which are mentioned at the end of Section 4.

# 2 The NNWR algorithm

Suppose we want to solve the 1D heat equation

$$\partial_t u - \partial_x^2 u = f, \qquad x \in \Omega = (-b, a), \quad t \in (0, T],$$

with initial conditions u(x,0) = v(x) and Dirichlet boundary conditions  $u(-b,t) = u_L(t)$ ,  $u(a,t) = u_R(t)$ . We consider a decomposition into two non-overlapping subdomains  $\Omega_1 = (-b,0)$  and  $\Omega_2 = (0,a)$ . On the interface  $\Gamma = \{0\}$ , we are given the initial guess  $g^0(t), t \in [0,T]$ . Then the NNWR algorithm is given by the following iteration: for k = 1, 2, ..., do

1. Dirichlet step:

$$\begin{cases} \partial_{t}u_{1}^{k} - \partial_{x}^{2}u_{1}^{k} = f(x,t) & \text{on} (-b,0), \\ u_{1}^{k}(-b,t) = u_{L}(t), & u_{1}^{k}(0,t) = g^{k-1}(t), \\ u_{1}^{k}(x,0) = v(x) & \text{on} (-b,0), \end{cases} \begin{cases} \partial_{t}u_{2}^{k} - \partial_{x}^{2}u_{2}^{k} = f(x,t) & \text{on} (0,a), \\ u_{2}^{k}(0,t) = g^{k-1}(t), & u_{2}^{k}(0,t) = g^{k-1}(t), \\ u_{2}^{k}(a,t) = u_{R}(t), & u_{2}^{k}(x,0) = v(x) & \text{on} (0,a). \end{cases}$$

2. Neumann step:

$$\begin{cases} \partial_t \psi_1^k - \partial_x^2 \psi_1^k = 0 & \text{on } (-b,0), \\ \psi_1^k (-b,t) = 0, & \\ \partial_{n_1} \psi_1^k = \partial_{n_1} u_1^k + \partial_{n_2} u_2^k & \text{on } \Gamma, \\ \psi_1^k (x,0) = 0 & \text{on } (-b,0), \end{cases} \begin{cases} \partial_t \psi_2^k - \partial_x^2 \psi_2^k = 0 & \text{on } (0,a), \\ \partial_{n_2} \psi_2^k = \partial_{n_1} u_1^k + \partial_{n_2} u_2^k & \text{on } \Gamma, \\ \psi_2^k (a,t) = 0, \\ \psi_2^k (x,0) = 0, & \text{on } (0,a). \end{cases}$$

3. Update step:

$$g^{k}(t) = g^{k-1}(t) - \theta[\psi_{1}^{k}(0,t) + \psi_{2}^{k}(0,t)]$$

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The relaxation parameter  $\theta \in (0, 1]$  is chosen to obtain fast convergence. Note that this algorithm can be generalized in a straightforward way to handle decompositions into many subdomains and in higher dimensions, see [10]. This is because, unlike for the elliptic case, the Neumann step is always well-posed for the heat equation, even for "floating" subdomains that do not share an edge with  $\partial \Omega$ .

Analysis by Laplace transforms. Our convergence analysis is based on the Laplace transform method. The Laplace transform of a function u(x,t) with respect to time is defined as

$$\hat{u}(x,s) := \mathscr{L}\{u(x,t)\} = \int_0^\infty u(x,t)e^{-st}\,dt.$$

In the remainder of the paper, hats will denote the Laplace transform of a function in time, and *s* will denote the Laplace variable. Since we are interested in the error  $g^k(t) - u(0,t)$  of the method, it suffices to assume that  $v(x), f(x,t), u_L(t)$  and  $u_R(t)$ all vanish and study how  $g^k(t)$  tends to zero as  $k \to \infty$ . In this case, the NNWR algorithm can be written in Laplace space as follows: for k = 1, 2, ..., do

1. Dirichlet step:

$$\begin{cases} (s - \partial_x^2) \hat{u}_1^k = 0 & \text{on } (-b, 0), \\ \hat{u}_1^k(-b, s) = 0, \\ \hat{u}_1^k(0, s) = \hat{g}^{k-1}(s), \end{cases} \begin{cases} (s - \partial_x^2) \hat{u}_2^k = 0 & \text{on } (0, a), \\ \hat{u}_2^k(0, s) = \hat{g}^{k-1}(s), \\ \hat{u}_2^k(a, t) = 0. \end{cases}$$
  
2. Neumann step:

$$\begin{cases} (s-\partial_x^2)\hat{\psi}_1^k = 0 & \text{ on } (-b,0), \\ \hat{\psi}_1^k(-b,s) = 0, & \\ \partial_x\hat{\psi}_1^k = \partial_x\hat{u}_1^k - \partial_x\hat{u}_2^k & \text{ on } \Gamma, \end{cases} \begin{cases} (s-\partial_x^2)\hat{\psi}_2^k = 0 & \text{ on } (0,a), \\ -\partial_x\hat{\psi}_2^k = \partial_x\hat{u}_1^k - \partial_x\hat{u}_2^k & \text{ on } \Gamma, \\ \hat{\psi}_2^k(a,s) = 0. \end{cases}$$

3. Update step:

$$\hat{g}^k(s) = \hat{g}^{k-1}(s) - \theta[\hat{\psi}_1^k(0,s) + \hat{\psi}_2^k(0,s)]$$

Solving the two-point boundary value problems in the Dirichlet step yields

$$\hat{u}_{1}^{k}(x,s) = \hat{g}^{k-1}(s)\frac{\sinh((x+b)\sqrt{s})}{\sinh(b\sqrt{s})}, \qquad \hat{u}_{2}^{k}(x,s) = \hat{g}^{k-1}(s)\frac{\sinh((a-x)\sqrt{s})}{\sinh(a\sqrt{s})}.$$
 (1)

The Neumann step can be solved similarly by letting  $\hat{r}^k(s) := \partial_x \hat{u}_1^k(0,s) - \partial_x \hat{u}_2^k(0,s)$ :

$$\hat{\psi}_1^k(x,s) = \hat{r}^k(s) \frac{\sinh((x+b)\sqrt{s})}{\sqrt{s}\cosh(b\sqrt{s})}, \qquad \hat{\psi}_2^k(x,s) = \hat{r}^k(s) \frac{\sinh((a-x)\sqrt{s})}{\sqrt{s}\cosh(a\sqrt{s})}.$$
 (2)

Then the update step becomes

$$\hat{g}^{k}(s) = \hat{g}^{k-1}(s) - \theta[\psi_{1}^{k}(0,s) + \psi_{2}^{k}(0,s)] = \hat{g}^{k-1}(s) - \theta \frac{\hat{r}^{k}(s)}{\sqrt{s}} [\tanh(b\sqrt{s}) + \tanh(a\sqrt{s})]$$

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$$\hat{r}^k(s) = \partial_x u_1^k(0,s) - \partial_x u_2^k(0,s) = \sqrt{s} \hat{g}^{k-1}(s) \left( \frac{\cosh(b\sqrt{s})}{\sinh(b\sqrt{s})} + \frac{\cosh(a\sqrt{s})}{\sinh(a\sqrt{s})} \right).$$

So we obtain

$$\hat{g}^{k}(s) = \hat{g}^{k-1}(s) \left[ 1 - \theta \left( 2 + \frac{\tanh(a\sqrt{s})}{\tanh(b\sqrt{s})} + \frac{\tanh(b\sqrt{s})}{\tanh(a\sqrt{s})} \right) \right].$$
(3)

Note that if a = b, then  $\hat{g}^k(s) = \hat{g}^{k-1}(s)(1-4\theta)$ , which means *the method converges* to the exact solution in one iteration for  $\theta = 1/4$ . Thus, the classical result for elliptic problems also holds for the time-dependent case. The main result of our paper concerns the case when the subdomains are unequal, i.e., when  $a \neq b$ .

**Theorem 1 (Convergence of NNWR).** Let  $\theta = 1/4$ . Then the error of the NNWR method for two subdomains satisfies

$$\|g^{k}(\cdot) - u(0, \cdot)\|_{L^{\infty}(0,\infty)} \le \left(\frac{(a-b)^{2}}{4ab}\right)^{k} \|g^{0}(\cdot) - u(0, \cdot)\|_{L^{\infty}(0,\infty)}.$$
 (4)

Moreover, for every finite time interval (0,T), NNWR converges superlinearly with the estimate

$$\|g^{k}(\cdot) - u(0, \cdot)\|_{L^{\infty}(0,T)} \le e^{-k^{2}m^{2}/T} \left(\frac{(a-b)^{2}}{ab}\right)^{k} \|g^{0}(\cdot) - u(0, \cdot)\|_{L^{\infty}(0,T)},$$
(5)

where  $m = \min\{a, b\}$ .

## **3** Convergence analysis

Since (3) is symmetric with respect to *a* and *b*, we will assume without loss of generality that a > b in the remainder of the paper. For  $\theta = 1/4$ , the recurrence (3) simplifies to give

$$\hat{g}^{k}(s) = -\hat{g}^{k-1}(s) \cdot \frac{\sinh^{2}((a-b)\sqrt{s})}{\sinh(2a\sqrt{s})\sinh(2b\sqrt{s})} =: -Y(s)\hat{g}^{k-1}(s), \tag{6}$$

which implies  $\hat{g}^k(s) = (-1)^k Y^k(s) \hat{g}^0(s)$ . Note that for  $\Re(s) > 0$ , we have  $Y(s) = O(e^{-4b|s|^{1/2}})$  as  $|s| \to \infty$ , i.e., Y(s) decays exponentially as  $|s| \to \infty$ . Thus, by [3, p. 183], Y(s) is the Laplace transform of a regular function  $y_1(t)$ . If we now define  $y_k(t) = \mathcal{L}^{-1}\{Y^k(s)\}$ , then for  $t \in (0, T)$ , we have

$$|g^{k}(t)| = \left| \int_{0}^{t} g^{0}(t-\tau) y_{k}(\tau) d\tau \right| \le ||g^{0}||_{L^{\infty}(0,T)} \int_{0}^{T} |y_{k}(\tau)| d\tau.$$
(7)

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Thus, to obtain  $L^{\infty}$  convergence estimates, we need bounds on  $\int_0^T |y_k(\tau)| d\tau$ . Our first step is to show that  $y_k(t) \ge 0$ , for t > 0, which makes bounding its integral much easier. We start by stating a few elementary properties of positive functions and their Laplace transforms; their proofs follow easily from the definitions.

**Lemma 1.** Let f and g be positive functions, i.e.,  $f(t) \ge 0$  and  $g(t) \ge 0$  for t > 0, and let  $F(s) = \mathcal{L}{f(t)}$ . Then

$$\begin{aligned} (i) \ For \ all \ T > 0, \ & \int_0^T |f(\tau)| \ d\tau \le \int_0^\infty f(\tau) \ d\tau = \lim_{s \to 0} F(s) \\ (ii) \ & (f * g)(t) = \int_0^t f(t - \tau)g(\tau) \ d\tau \ge 0 \ for \ all \ t > 0. \\ (iii) \ & \|f * g\|_{L^1(0,T)} \le \|f\|_{L^1(0,T)} \cdot \|g\|_{L^1(0,T)}. \end{aligned}$$

**Lemma 2.** For  $\beta > \alpha \ge 0$ , let

$$Q_1(s) = \frac{\sinh(\alpha\sqrt{s})}{\sinh(\beta\sqrt{s})}, \qquad Q_2(s) = \frac{\cosh(\alpha\sqrt{s})}{\cosh(\beta\sqrt{s})}.$$

Then  $q_1(t) = \mathscr{L}^{-1}{Q_1(s)}$  and  $q_2(t) = \mathscr{L}^{-1}{Q_2(s)}$  are positive functions.

*Proof.* For  $n = 1, 2, ..., let u_n(x, t)$  and  $v_n(x, t)$  be the solutions of the following two boundary value problems:

$$\begin{cases} \partial_t u_n - \partial_x^2 u_n = 0 & \text{on } (0, \beta), \\ u_n(0, t) = 0, \\ u_n(\beta, t) = f_n(t), \\ u_n(x, 0) = 0, \end{cases} \begin{cases} \partial_t w_n - \partial_x^2 w_n = 0 & \text{on } (-\beta, \beta), \\ w_n(-\beta, t) = f_n(t), \\ w_n(\beta, t) = f_n(t), \\ w_n(x, 0) = 0. \end{cases}$$

A calculation similar to that in Section 2 shows that  $\mathscr{L}\{u_n(\alpha,t)\} = Q_1(s)\hat{f}_n(s)$  and  $\mathscr{L}\{w_n(\alpha,t)\} = Q_2(s)\hat{f}_n(s)$ . Moreover, if  $f_n(t) \ge 0$  for all *t*, then by the maximum principle, we have  $u_n(\alpha,t) \ge 0$ . We now choose a sequence  $(f_n)$  of positive functions that converges weakly to  $\delta(t)$ ; then since each  $u_n(\alpha,t)$  is positive, we have  $u_n(\alpha,t) \to q_1(t) \ge 0$ . A similar argument shows that  $w_n(\alpha,t) \to q_2(t) \ge 0$ .  $\Box$ 

We now analyze the kernel  $y_1(t)$ , with Laplace transform Y(s), as defined in (6).

**Lemma 3.** Let  $m \ge 1$  be the unique integer such that  $mb < a \le (m+1)b$ . Then Y(s) = V(s)H(s), with  $V(s) = 1/\cosh^2(b\sqrt{s})$  and  $\lim_{s\to 0} H(s) = (a-b)^2/4ab$ . Moreover,  $h(t) = \mathcal{L}^{-1}{H(s)}$  is positive, so that  $y_1(t) = (v * h)(t) \ge 0$  for all t > 0.

*Proof.* For k < m, we have the identity

$$\begin{aligned} \sinh^2((a-kb)\sqrt{s}) - \sinh^2((a-(k+1)b)\sqrt{s}) \\ &= \frac{1}{2} \left[ \cosh(2(a-kb)\sqrt{s}) - 1 - \cosh(2(a-(k+1)b)\sqrt{s}) + 1 \right] \\ &= \sinh((2a-(2k+1)b)\sqrt{s})\sinh(b\sqrt{s}). \end{aligned}$$

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Since k < m, we have 0 < 2a - (2k+1)b < 2a, which gives

$$\frac{\sinh^2((a-kb)\sqrt{s})}{\sinh(2a\sqrt{s})\sinh(2b\sqrt{s})} = \frac{\sinh((2a-(2k+1)b)\sqrt{s})}{\sinh(2a\sqrt{s})} \cdot \frac{\sinh(b\sqrt{s})}{\sinh(2b\sqrt{s})} + \frac{\sinh^2((a-(k+1)b)\sqrt{s})}{\sinh(2a\sqrt{s})\sinh(2b\sqrt{s})}$$

Applying this identity repeatedly for k = 1, ..., m - 1 gives

Let  $V(s) = 1/\cosh^2(b\sqrt{s})$  and H(s) be the rest. Then since  $0 < a - mb \le b < a$ , we see that H(s) consists of a sum of products of functions of the form  $Q_1(s)$  and  $Q_2(s)$  in Lemma 2. Thus, its inverse Laplace transform h(t) is positive. Moreover, since  $v(t) = \mathcal{L}^{-1}{V(s)}$  is also positive by Lemma 2, we see that y(t) = (v \* h)(t)is positive. Finally, since  $\lim_{s\to 0} V(s) = 1$ , we have

$$\lim_{s \to 0} H(s) = \lim_{s \to 0} Y(s) = \lim_{s \to 0} \frac{\sinh^2((a-b)\sqrt{s})}{\sinh(2a\sqrt{s})\sinh(2b\sqrt{s})} = \frac{(a-b)^2}{4ab}.$$

We are finally ready to prove our main result.

*Proof (Theorem 1).* According to (7), it suffices to bound  $\int_0^T |y_k(\tau)| d\tau$  for finite T > 0 and for  $T = \infty$ , where  $y_k(t) = \mathcal{L}^{-1}{Y^k(s)}$ . Since  $y_1(t)$  is positive by Lemma 3, so is  $y_k(t)$ , so by Lemma 1(i), we have

$$\int_0^\infty |y_k(\tau)| d\tau = \lim_{s \to 0} Y^k(s) = \left(\frac{(a-b)^2}{4ab}\right)^k,$$

which shows the linear bound (4). For  $T < \infty$ , let  $v_k(t) = \mathscr{L}^{-1}\{V^k(s)\}$  and  $h_k(t) = \mathscr{L}^{-1}\{H^k(s)\}$ . Then since  $\int_0^\infty h_k(t) dt = \lim_{s \to 0} H^k(s) = (\lim_{s \to 0} H(s))^k$ , we have

$$\|y_k\|_{L^1(0,T)} \le \|v_k\|_{L^1(0,T)} \cdot \|h_k\|_{L^1(0,T)} \le \left(\frac{(a-b)^2}{4ab}\right)^k \int_0^T v_k(\tau) \, d\tau.$$
(8)

To bound the remaining integral, let  $D(s) = 4^k e^{-2kb\sqrt{s}} - V^k(s)$ . We will show that  $d(t) = \mathcal{L}^{-1}\{D(s)\} \ge 0$ . We have

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$$D(s) = 4^{k}e^{-2kb\sqrt{s}} - \frac{2^{2k}}{(e^{b\sqrt{s}} + e^{-b\sqrt{s}})^{2k}} = 4^{k} \cdot \frac{(1 + e^{-2b\sqrt{s}})^{2k} - 1}{(e^{b\sqrt{s}} + e^{-b\sqrt{s}})^{2k}} = 4^{k}\sum_{m=1}^{2k} \binom{2k}{m}e^{-2bm\sqrt{s}}V^{k}(s)$$

From [17], we know that  $\mathscr{L}^{-1}\{e^{-2bm\sqrt{s}}\} = \frac{bm}{\sqrt{\pi t^3}}e^{-b^2m^2/t}$  is a positive function for  $m \ge 1$ . Since  $v_k(t) = \mathscr{L}^{-1}\{V^k(s)\}$  is also positive, we see that d(t) is in fact a sum of convolutions of positive functions. Hence  $d(t) \ge 0$ , as claimed. Thus, we have

$$\int_0^T v_k(\tau) d\tau \le \int_0^T (v_k(\tau) + d(\tau)) d\tau = \int_0^T 4^k \frac{kb}{\sqrt{\pi\tau^3}} e^{-k^2b^2/\tau} d\tau = 4^k \operatorname{erfc}\left(\frac{bk}{\sqrt{T}}\right).$$

But  $\operatorname{erfc}(x) \le e^{-x^2}$  for all  $x \ge 0$ ; introducing this into (8) gives the estimate

$$\|y_k\|_{L^1(0,T)} \leq \left(\frac{(a-b)^2}{ab}\right)^k \operatorname{erfc}\left(\frac{bk}{\sqrt{T}}\right) \leq \left(\frac{(a-b)^2}{ab}\right)^k e^{-k^2b^2/T},$$

which tends to zero as  $k \to \infty$ .

### **4** Numerical experiments

Figure 1 shows the convergence of NNWR for a mildly asymmetric case (a = 0.7, b = 0.3) and a strongly asymmetric case (a = 0.9, b = 0.1) when applied to a finitedifference Crank–Nicolson discretization. We see that the bounds in Theorem 1, while not necessarily sharp, does capture the superlinear convergence of the method. As the length of the time window *T* increases, the error curve approaches the linear bound, which can be increasing for highly asymmetric problems. In this case, the error can grow substantially before decreasing to zero superlinearly. Thus, one should divide up the problem into several small time windows before using NNWR.



**Fig. 1** Convergence curves and their respective bounds for (i) a = 0.7, b = 0.3 and (ii) a = 0.9, b = 0.1. The solid curves (with markers) denote the  $L^{\infty}$  error after k iterations for the final time T indicated, and dotted lines of the same color show the superlinear bound (5) for the same T. The linear bound (4) is shown as a solid black line (no markers).

Convergence estimates for more general decompositions can also be obtained. For the 1D heat equation with *N* subdomains, we have

$$\max_{1 \le i \le N} \|e_i^k\|_{L^{\infty}(0,T)} \le \left(\frac{\sqrt{6}}{1 - e^{-(2k+1)/\tau}}\right)^{2k} e^{-k^2/\tau} \max_{1 \le i \le N} \|e_i^0\|_{L^{\infty}(0,T)},\tag{9}$$

where  $e_i^k$  is the error along the *i*th interface at iteration k and  $\tau = T/h^2$ , with h being the smallest subdomain size. The estimate (9) is also valid for the 2D heat equation on a rectangular domain decomposed into N strips. For the proofs of these and other results, see [10]. Note that as N increases, the subdomain size h necessarily decreases, and the bound (9) shows that the error can increase before superlinear convergence kicks in, just like in the asymmetric case above. To remedy this, we recommend using a coarse grid correction, which is the subject of a future paper.

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