# A Waveform Relaxation Algorithm with Overlapping Splitting for Reaction Diffusion Equations

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Waveform relaxation is a technique to solve large systems of ordinary differential equations (ODEs) in parallel. The right hand side of the system is split into subsystems which are only loosely coupled. One then solves iteratively all the subsystems in parallel and exchanges information after each step of the iteration. Two classical convergence results state linear convergence on unbounded time intervals for linear systems of ODEs under some dissipation assumption and superlinear convergence on bounded time intervals for nonlinear systems under a Lipschitz condition on the splitting.

To apply waveform relaxation to partial differential equations (PDEs), one traditionally discretizes the PDE in space to get a large system of ODEs, to which then the waveform relaxation algorithm is applied using a matrix splitting. There are two problems with this approach: first information about how to split the right hand side is lost during the discretization; second the convergence results derived in this fashion depend in general on the mesh parameter and convergence rates deteriorate when the mesh is refined. To avoid those problems a new waveform relaxation algorithm is formulated directly at the PDE level. The differential operator on the right hand side is split using domain decomposition. It is shown for a scalar reaction diffusion equation with variable diffusion coefficient that the new waveform relaxation algorithm converges superlinearly for bounded time intervals and linearly for unbounded time intervals, extending the two classical convergence results to this type of PDE. Interestingly the superlinear convergence rate is faster than the superlinear convergence rate obtained by the traditional matrix splitting methods. It is shown how the convergence rates depend on the overlap of the domain decomposition and a Lipschitz condition on the reaction function. The splitting of the right hand side is naturally given by the domain decomposition and the convergence rates are robust with respect to mesh refinement when the algorithm is discretized.

KEY WORDS Waveform Relaxation, Domain Decomposition, Reaction Diffusion Equations, Overlapping Splitting

#### 1. Introduction

The basic ideas of waveform relaxation were introduced in the late 19th century by Picard [24] and Lindelöf [15] to study initial value problems. There has been much recent interest in waveform relaxation as a practical method for the solution of stiff ordinary differential equations (ODEs) after the publication of a paper by Lelarasmee, Ruehli and Sangiovanni-Vincentelli [14] in the area of circuit simulation. For some problems there is even a speedup for the sequential version of the algorithm, but the real interest lies in the inherent paral-

lelism of waveform relaxation methods, making them attractive for large scale applications ([27], [13], [23], [18], [4]).

There are two basic types of convergence results for waveform relaxation algorithms for ODEs: (i) for linear systems of ODEs on unbounded time intervals one can show linear convergence of the algorithm under some dissipation assumptions on the splitting ([19], [20,21], [12] and [4]); (ii) for nonlinear systems of ODEs (including linear ones) on bounded time intervals one can show superlinear convergence assuming a Lipschitz condition on the splitting function ([20,21], [2] and [3]). For classical relaxation methods (Jacobi, Gauss Seidel, SOR) the above convergence results depend on the discretization parameter if the ODE arises from a PDE which is discretized in space. The convergence rates deteriorate as one refines the mesh and thus makes the methods unpractical.

Mesh dependence can be overcome using multigrid. Lubich and Osterman prove in [17] linear convergence for the one dimensional heat equation independent of the mesh parameter. Their analysis based on an eigenvector approach however is not easily generalizable [4]. A more general approach to analyze multi grid waveform relaxation was given by Ta'asan and Zhang [26]. Further results can be found in Janssen and Vandewalle [11].

Another way of overcoming mesh dependence is by formulating the waveform relaxation using Schwarz overlapping domain decomposition. This was done simultaneously and independently by Gander and Stuart [8] who established results of type (i) and by Giladi and Keller [10] who established results of type (ii), both for dissipative linear PDEs. We call this type of algorithms overlapping Schwarz waveform relaxation.

In this paper we extend the linear and superlinear convergence results established in [8] and [10] for overlapping Schwarz waveform relaxation to nonlinear parabolic equations of reaction diffusion type with variable diffusion coefficient. The main tool in the analysis is a Positivity Lemma, which is established in Section 2. In Section 3. we formulate the overlapping Schwarz waveform relaxation algorithm for the reaction diffusion equation. In Section 4. we prove linear convergence of the algorithm on unbounded time intervals at the continuous level provided the growth of the reaction function is bounded by the smallest eigenvalue of the Laplacian. In Section 5. we prove superlinear convergence of the algorithm on bounded time intervals assuming the growth of the reaction function is bounded from above by any finite constant. In Section 6. we generalize the results of Sections 4. and 5. to the case where the diffusion coefficient varies in space and time. Numerical experiments which support the convergence analysis are presented in Section 7. In the last section we show how our estimates can be sharpened using a local argument. We also show how the analysis can be generalized to several subdomains leading to an inherently parallel algorithm. We conclude by an outlook on how the present analysis could be extended to higher dimensional problems.

#### 2. The Positivity Lemma

The Positivity Lemma is central in our analysis of the overlapping Schwarz waveform relaxation algorithm for reaction diffusion equations. It's proof can be found for example for bounded time domains in [22], where the result is deduced from a Maximum Principle. We give here a simple direct proof valid for unbounded time domains as well.

**Lemma 2.1. (Positivity Lemma)** Suppose the function  $w \in C([0, L] \times [0, \infty]) \cap C^{2,1}((0, L) \times [0, \infty])$ 

 $(0,\infty)$ ) satisfies the differential inequalities

$$\frac{\partial w}{\partial t} - c^{2}(x, t) \frac{\partial^{2} w}{\partial x^{2}} + a(x, t)w \geq 0 \qquad 0 < x < L, \ t > 0$$

$$w(0, t) \geq 0 \qquad t > 0$$

$$w(L, t) \geq 0 \qquad t > 0$$

$$w(x, 0) \geq 0 \qquad 0 \leq x \leq L,$$
(2.1)

where a(x,t) is a function bounded from below,  $a(x,t) \geq C$  for some constant C and  $c^2(x,t) > 0$  for all  $x \in (0,L)$  and  $t \in (0,\infty)$ . Then

$$w(x,t) > 0 \quad \forall x \in [0,L], t \in [0,\infty).$$

Proof Consider the case first where the function a(x,t) is strictly positive, a(x,t)>0 for all  $x\in(0,L)$  and  $t\in(0,\infty)$ . To reach a contradiction, suppose that the function w(x,t) becomes negative,  $w(x,t)\leq -\delta<0$  for some positive quantity  $\delta$  and some  $x,t\in(0,L)\times(0,\infty)$ . By continuity there exists a first time  $t_0$  and a point  $x_0$  where w reaches the value  $-\frac{\delta}{2}, w(x_0,t_0)=-\frac{\delta}{2}$ . Then the time derivative of w at that point is non-positive,  $w_t(x_0,t_0)\leq 0$  and the second spatial derivative is non-negative,  $w_{xx}(x_0,t_0)\geq 0$ , since otherwise there would be a point nearby  $(x_0,t_0)$  at which w is already smaller than  $-\frac{\delta}{2}$ . But w satisfies the differential inequality (2.1),

$$w_t(x_0, t_0) - c^2(x, t)w_{xx}(x_0, t_0) + a(x_0, t_0)w(x_0, t_0) \ge 0,$$

which is a contradiction, since the first term is non positive, the second non-negative and the third one strictly negative. Therefore the function w can not become negative in the interior of the domain. But on the boundary, it is non-negative by definition and thus the result follows. Now for general functions a(x,t) which are bounded from below, a(x,t)>C, consider the function  $v:=e^{Ct}w$ . This function satisfies the differential inequality

$$v_t - c^2(x, t)v_{xx} + (a(x, t) - C)v > 0,$$

with non-negative initial and boundary data. Because a(x,t) is bounded from below by C we have a(x,t)-C>0 and hence by the above argument v can not become negative. This implies that w cannot become negative either, since  $w=e^{-Ct}v$ , which concludes the proof.

**Remark:** It suffices for w to be piecewise continuous at the boundary for the Lemma to hold, since the continuity at the boundary was not used in the proof.

All the convergence results we obtain in this paper are for continuous problems and depend on the Positivity Lemma. An identical convergence analysis applies to the semi discrete equations, as it was shown for the heat equation in [8], provided we have a discrete Positivity Lemma. For completeness we present here a discrete Positivity Lemma for a finite difference discretization.

Suppose the inequalities (2.1) have been discretized by a centered finite difference scheme on a grid with n gridpoints, h = L/(n+1). Then setting  $a_j(t) := a(jh, t)$  and  $c_j(t) := c(jh, t)$  for  $j = 1, 2, \ldots, n$  we get the set of discrete ODE inequalities

$$\frac{d\boldsymbol{w}}{dt} \ge A(t)\boldsymbol{w} \tag{2.2}$$

where the matrix A(t) is given by

$$A(t) = \frac{1}{h^2} \begin{bmatrix} -2c_1(t) - a_1(t)h^2 & c_1(t) \\ c_2(t) & -2c_2(t) - a_2(t)h^2 & c_2(t) \\ & \ddots & \ddots \\ c_n(t) & -2c_n(t) - a_n(t)h^2 \end{bmatrix}$$
(2.3)

and the initial condition  $w(0) \ge 0$ . Note that all the inequalities are componentwise.

**Lemma 2.2. (Discrete Positivity Lemma)** Suppose  $c_j(t)$  and  $a_j(t)$  are bounded for all t > 0 and  $1 \le j \le n$ . Then

$$w(t) \ge 0 \quad \forall t \in [0, \infty).$$

*Proof* Using an integrating factor in (2.2) we obtain

$$\boldsymbol{w}(t) \geq e^{\int_0^t A(s)ds} \boldsymbol{w}(0)$$

Now defining  $C := \sup_{j,t} (2c_j(t)/h^2 + a_j(t))$  and denoting the identity matrix by I, the exponential can be split into a scalar factor and the exponential of a matrix with non negative entries only,

$$\boldsymbol{w}(t) \ge e^{-Ct} e^{\int_0^t A(s) + CIds} \boldsymbol{w}(0).$$

Thus  $w(t) \ge 0$  since  $w(0) \ge 0$ .

#### 3. The Overlapping Schwarz Waveform Relaxation Algorithm

We consider the one dimensional reaction diffusion equation on the domain  $\Omega = [0, L] \times [0, T)$ ,

$$\begin{array}{rcl} \frac{\partial u}{\partial t} & = & c^2(x,t) \frac{\partial^2 u}{\partial x^2} + f(u) & & 0 < x < L, \ 0 < t < T \\ u(0,t) & = & g_1(t) & & 0 < t < T \\ u(L,t) & = & g_2(t) & & 0 < t < T \\ u(x,0) & = & u_0(x) & & 0 \le x \le L \end{array} \tag{3.1}$$

with  $f \in C^1(\mathbb{R})$  and  $\underline{c}^2 \leq c^2(x,t) \leq \overline{c}^2$  for  $0 \leq x \leq L$  and 0 < t < T. We assume that f'(u) < C for a finite constant C and that the given data  $g_1(t)$ ,  $g_2(t)$  and  $u_0(t)$  are piecewise continuous. This gives existence and uniqueness of a solution to (3.1) [22].

To obtain a waveform relaxation algorithm for (3.1) we decompose the domain  $\Omega$  into two overlapping subdomains  $\Omega_1 = [0, \beta L] \times [0, T)$  and  $\Omega_2 = [\alpha L, L] \times [0, T)$  where  $0 < \alpha < \beta < 1$  as given in Figure 1. We define two subproblems

$$\frac{\partial v}{\partial t} = c^2(x,t)\frac{\partial^2 v}{\partial x^2} + f(v) \qquad 0 < x < \beta L, \ 0 < t < T 
v(0,t) = g_1(t) \qquad 0 < t < T 
v(\beta L,t) = w(\beta L,t) \qquad 0 < t < T 
v(x,0) = u_0(x) \qquad 0 \le x \le \beta L$$
(3.2)

and

$$\frac{\partial w}{\partial t} = c^{2}(x,t)\frac{\partial^{2}w}{\partial x^{2}} + f(w) \qquad \alpha L < x < L, \ 0 < t < T 
w(\alpha L, t) = v(\alpha L, t) \qquad 0 < t < T 
w(L, t) = g_{2}(t) \qquad 0 < t < T 
w(x, 0) = u_{0}(x) \qquad \alpha L \le x \le L.$$
(3.3)

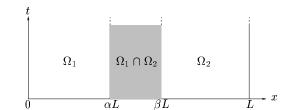


Figure 1. Decomposition into two overlapping subdomains.

Note that setting v(x,t) := u(x,t) on  $\Omega_1$  and w(x,t) := u(x,t) on  $\Omega_2$  is a solution to (3.2) and (3.3). A waveform relaxation algorithm to obtain this solution can be formulated using a Schwarz type iteration introduced for elliptic problems in [25] and further studied in [16], [6] and references therein. In the parabolic case, we obtain the overlapping Schwarz waveform relaxation algorithm

and

$$\frac{\partial w^{k+1}}{\partial t} = c^{2}(x,t)\frac{\partial^{2}w^{k+1}}{\partial x^{2}} + f(w^{k+1}) \qquad \alpha L < x < L, \ 0 < t < T 
w^{k+1}(\alpha L,t) = v^{k}(\alpha L,t) \qquad 0 < t < T 
w^{k+1}(L,t) = g_{2}(t) \qquad 0 < t < T 
w^{k+1}(x,0) = u_{0}(x) \qquad \alpha L \le x \le L.$$
(3.5)

To analyze the convergence of this algorithm to the solution u(x,t), define the errors on the subdomains  $d^k(x,t) := v^k(x,t) - u(x,t)$  and  $e^k(x,t) := w^k(x,t) - u(x,t)$  and consider the error equations

and

where we have used the remainder term in Taylors theorem,

$$f(v^{k+1}) - f(u) = f'(\xi^{k+1})d^{k+1}$$

for some function  $\xi^{k+1}(x,t)$  which lies between  $v^{k+1}(x,t)$  and u(x,t) for  $0 \le x \le \beta L$ , 0 < t < T, and similarly

$$f(w^{k+1}) - f(u) = f'(\eta^{k+1})e^{k+1}$$

for some function  $\eta^{k+1}(x,t)$  which lies between  $w^{k+1}(x,t)$  and u(x,t) for  $\alpha L \leq x \leq L$ , 0 < t < T.

We first consider the case where the diffusion coefficient is constant,  $c^2(x,t) \equiv c^2$ . The case with variable diffusion is investigated in Section 6.

# 4. Linear Convergence on Unbounded Time Intervals

We prove linear convergence of the overlapping Schwarz waveform relaxation algorithm (3.4) and (3.5) on unbounded time intervals,  $T=\infty$ . We consider in the following functions in  $L^{\infty}:=L^{\infty}({\rm IR}^+;{\rm IR})$  with the infinity norm

$$||f(\cdot)||_{\infty} := \sup_{t>0} |f(t)|.$$

**Lemma 4.1.** Suppose that the derivative of f in (3.1) is uniformly bounded from above by a constant  $a < \left(\frac{c\pi}{L}\right)^2$ . Then the error in the iteration (3.6), (3.7) decays linearly on the interfaces  $x = \alpha L$  and  $x = \beta L$ . Specifically

$$||d^{k+2}(\alpha L, \cdot)||_{\infty} \leq \gamma ||d^k(\alpha L, \cdot)||_{\infty}, \tag{4.1}$$

$$||e^{k+2}(\beta L, \cdot)||_{\infty} \leq \gamma ||e^{k}(\beta L, \cdot)||_{\infty}, \tag{4.2}$$

where the factor  $\gamma \in (0,1)$  is given by

$$\gamma = \left(\frac{\sin(\frac{\sqrt{a}}{c}(1-\beta)L)}{\sin(\frac{\sqrt{a}}{c}(1-\alpha)L)}\right) \left(\frac{\sin(\frac{\sqrt{a}}{c}\alpha L)}{\sin(\frac{\sqrt{a}}{c}\beta L)}\right). \tag{4.3}$$

*Proof* Consider the differential equation

$$\frac{\partial \tilde{d}^{k+2}}{\partial t} = c^2 \frac{\partial^2 \tilde{d}^{k+2}}{\partial x^2} + a\tilde{d}^{k+2} \qquad 0 < x < \beta L, \ t > 0 
\tilde{d}^{k+2}(0,t) = 0 \qquad t > 0 
\tilde{d}^{k+2}(\beta L,t) = ||e^{k+1}(\beta L,\cdot)||_{\infty} \qquad t > 0 \qquad (4.4)$$

$$\tilde{d}^{k+2}(x,0) = ||e^{k+1}(\beta L,\cdot)||_{\infty} \frac{\sin(\frac{\sqrt{a}}{c}x)}{\sin(\frac{\sqrt{a}}{c}\beta L)} \quad 0 \le x \le \beta L.$$

The solution to (4.4) is the steady state solution

$$\tilde{d}^{k+2}(x) = ||e^{k+1}(\beta L, \cdot)||_{\infty} \frac{\sin(\frac{\sqrt{a}}{c}x)}{\sin(\frac{\sqrt{a}}{\beta}L)}.$$
(4.5)

Note that  $\tilde{d}^{k+2}(x)$  is non-negative for  $0 \le x \le \beta L$  since  $-\infty < a \le \left(\frac{c\pi}{L}\right)^2$ . Hence the difference  $w := \tilde{d}^{k+2} - d^{k+2}$  satisfies

$$\frac{\partial w}{\partial t} = c^2 \frac{\partial^2 w}{\partial x^2} + a\tilde{d}^{k+2} - f'(\xi^{k+2})d^{k+2} \qquad 0 < x < \beta L, \ t > 0$$

$$w(0,t) = 0 \qquad \qquad t > 0$$

$$w(\beta L,t) \geq 0 \qquad \qquad t > 0$$

$$w(x,0) \geq 0 \qquad 0 \leq x \leq \beta L.$$
(4.6)

To apply the Positivity Lemma, note that the term on the right hand side in (4.6) can be written as

$$\begin{array}{lcl} a\tilde{d}^{k+2} - f'(\xi^{k+2})d^{k+2} & = & a\tilde{d}^{k+2} - f'(\xi^{k+2})\tilde{d}^{k+2} + f'(\xi^{k+2})\tilde{d}^{k+2} - f'(\xi^{k+2})d^{k+2} \\ & = & (a - f'(\xi^{k+2}))\tilde{d}^{k+2} + f'(\xi^{k+2})w. \end{array}$$

Now using the fact that  $\tilde{d}^{k+2}$  is non-negative and the assumption that f' is bounded by a, the first term on the right is non-negative and therefore the partial differential equation in (4.6) can be replaced by a differential inequality, namely

$$\frac{\partial w}{\partial t} - c^2 \frac{\partial^2 w}{\partial x^2} - f'(\xi^{k+2}) w \ge 0, \quad 0 < x < \beta L, \ t > 0.$$

Now the Positivity Lemma applies so that  $w=\tilde{d}^{k+2}-d^{k+2}\geq 0$ . A similar argument holds for the sum  $\tilde{w}:=\tilde{d}^{k+2}+d^{k+2}\geq 0$ , and thus the modulus of  $d^{k+2}(x,t)$  can be bounded by

$$|d^{k+2}(x,t)| \le \tilde{d}^{k+2}(x) = ||e^{k+1}(\beta L, \cdot)||_{\infty} \frac{\sin(\frac{\sqrt{a}}{c}x)}{\sin(\frac{\sqrt{a}}{c}\beta L)}.$$
(4.7)

Similarly on the second subdomain

$$|e^{k+1}(x,t)| \le ||d^k(\alpha L, \cdot)||_{\infty} \frac{\sin(\frac{\sqrt{a}}{c}(L-x))}{\sin(\frac{\sqrt{a}}{c}(1-\alpha)L)}$$

$$(4.8)$$

Evaluating this last equation at  $x = \beta L$ , taking the supremum over all t > 0 and inserting the result into equation (4.7) leads to the inequality

$$|d^{k+2}(x,t)| \le ||d^k(\alpha L,\cdot)||_{\infty} \left( \frac{\sin(\frac{\sqrt{a}}{c}(1-\beta)L)}{\sin(\frac{\sqrt{a}}{c}(1-\alpha)L)} \right) \left( \frac{\sin(\frac{\sqrt{a}}{c}x)}{\sin(\frac{\sqrt{a}}{c}\beta L)} \right). \tag{4.9}$$

Now evaluate (4.9) at  $x = \alpha L$  and take the supremum over t > 0 to obtain

$$||d^{k+2}(\alpha L, \cdot)||_{\infty} \le \gamma ||d^k(\alpha L, \cdot)||_{\infty},$$

with  $\gamma$  as given in (4.3). The second inequality is obtained similarly. It remains to show that with the given condition on a the convergence factor  $\gamma < 1$ . Consider the cases a=0, a<0 and  $0< a<\left(\frac{c\pi}{L}\right)^2$  separately. For a=0 the result for the heat equation obtained in [8] is recovered, namely

$$\lim_{a \to 0} \gamma = \frac{\alpha(1-\beta)}{\beta(1-\alpha)},\tag{4.10}$$

which is clearly less than 1 for  $0 < \alpha < \beta < 1$ . For a < 0 the factor  $\gamma$  can be rewritten as

$$\gamma = \frac{\coth(\frac{\sqrt{|a|}}{c}\beta L) - \coth(\frac{\sqrt{|a|}}{c}L)}{\coth(\frac{\sqrt{|a|}}{c}\alpha L) - \coth(\frac{\sqrt{|a|}}{c}L)}.$$
(4.11)

Noting that  $\coth(x)$  is monotonically decreasing for x>0 and using the fact that  $0<\alpha<\beta<1$  one obtains  $\gamma<1$  for a<0. In the last case,  $0< a<\left(\frac{c\pi}{L}\right)^2$ , rewrite  $\gamma$  in the form

$$\gamma = \frac{\cot(\frac{\sqrt{a}}{c}\beta L) - \cot(\frac{\sqrt{a}}{c}L)}{\cot(\frac{\sqrt{a}}{c}\alpha L) - \cot(\frac{\sqrt{a}}{c}L)}.$$
(4.12)

Noting that  $\cot(x)$  is monotonically decreasing for  $0 < x < \pi$  and using  $0 < \alpha < \beta < 1$  one obtains again  $\gamma < 1$  for  $0 < a < \left(\frac{c\pi}{L}\right)^2$ . Hence  $\gamma < 1$  for  $a < \left(\frac{c\pi}{L}\right)^2$  and the proof is established.

For any function g(x,t) in  $L^{\infty}([a,b],L^{\infty})$  we introduce the norm

$$|||g(\cdot,\cdot)|||_{\infty} := \sup_{a \le x \le b} ||g(x,\cdot)||_{\infty}.$$

**Theorem 4.1. (Linear Convergence)** Assume that the derivative of f in (3.1) is uniformly bounded from above by a constant  $a < \left(\frac{c\pi}{L}\right)^2$ . Then the overlapping Schwarz waveform relaxation algorithm for the reaction diffusion equation (3.1) with two subdomains converges linearly for any initial guess at a rate depending on the size of the overlap and the ratio of the constant a to the diffusion coefficient  $c^2$ . Specifically

$$|||d^{2k+1}(\cdot,\cdot)|||_{\infty} \le \gamma^k C_1 ||e^0(\beta L,\cdot)||_{\infty}$$
 (4.13)

$$|||e^{2k+1}(\cdot,\cdot)|||_{\infty} \le \gamma^k C_2 ||d^0(\alpha L,\cdot)||_{\infty},$$
 (4.14)

where

$$\gamma = \left(\frac{\sin(\frac{\sqrt{a}}{c}(1-\beta)L)}{\sin(\frac{\sqrt{a}}{c}(1-\alpha)L)}\right) \left(\frac{\sin(\frac{\sqrt{a}}{c}\alpha L)}{\sin(\frac{\sqrt{a}}{c}\beta L)}\right). \tag{4.15}$$

and the constants  $C_1$  and  $C_2$  are given by

$$C_{1} = \sup_{0 < x < \beta L} \frac{\sin(\frac{\sqrt{a}}{c}x)}{\sin(\frac{\sqrt{a}}{c}\beta L)}$$

$$C_{2} = \sup_{\alpha L < x < L} \frac{\sin(\frac{\sqrt{a}}{c}(L-x))}{\sin(\frac{\sqrt{a}}{c}(1-\alpha)L)}.$$

$$(4.16)$$

*Proof* From equation (4.7) in the proof of Lemma 4.1. one obtains

$$|d^{2k+1}(x,t)| \le ||e^{2k}(\beta L,\cdot)||_{\infty} \frac{\sin(\frac{\sqrt{a}}{c}x)}{\sin(\frac{\sqrt{a}}{c}\beta L)}.$$
(4.17)

Using Lemma 4.1. for  $||e^{2k}(\beta L, \cdot)||_{\infty}$  in (4.17) and taking the supremum in x on the right leads to

$$|d^{2k+1}(x,t)| \le C_1 \gamma^k ||e^0(\beta L, \cdot)||_{\infty}$$

which is the desired uniform bound in x and t. The second inequality is obtained analogously.

We now analyze how the rate of convergence  $\gamma$  depends on the size of the overlap determined by the parameters  $\alpha$  and  $\beta$  and on the constants a and  $c^2$  given in the problem. First note that for  $a=\left(\frac{c\pi}{L}\right)^2$  the iteration factor becomes

$$\gamma = \frac{\sin(\pi(1-\beta))}{\sin(\pi(1-\alpha))} \frac{\sin(\pi\alpha)}{\sin(\pi\beta)} = 1.$$

The last step follows from the identity  $\sin(a-b)=\sin(a)\cos(b)-\cos(a)\sin(b)$ . Hence the iteration stagnates for  $a=\left(\frac{c\pi}{L}\right)^2$ . For  $a<\left(\frac{c\pi}{L}\right)^2$  Figure 2 shows how  $\gamma$  depends on a for L=1 and  $\alpha=0.4$ ,  $\beta=0.6$  and  $c^2=1$ . The graph depicts clearly that the convergence of

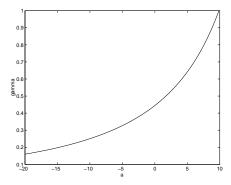


Figure 2. Dependence of the iteration factor  $\gamma$  on the constant a given by the problem

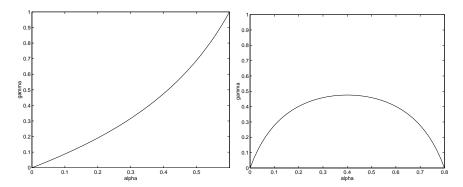


Figure 3. Dependence of the iteration factor  $\gamma$  on the overlap size on the left (fixed  $\beta$ ) and on the position of the overlap (fixed  $\beta - \alpha$ ) on the right for a = 1

the algorithm becomes faster the smaller a is. This agrees with the intuition that the smaller a is the faster the solution decays. In fact from (4.11)

$$\lim_{a\to -\infty}\gamma=0.$$

Note that a small diffusion coefficient  $c^2$  amplifies the effect of a.

The dependence on the overlap is shown in Figure 3. On the left the size of the overlap is varied by fixing  $\beta=0.6$  and varying  $\alpha\in[0,0.6]$ . Clearly the iteration converges faster if the overlap is increased by decreasing  $\alpha$ . On the other hand, if the overlap approaches zero, the convergence factor becomes, using (4.3)

$$\lim_{\alpha\to\beta}\gamma=1$$

and thus the algorithm does not converge without overlap. This agrees with intuition as well, since without overlap, no information is exchanged.

In Figure 3 on the right the size of the overlap  $\beta-\alpha\equiv 0.2$  is fixed and the overlap is moved across the domain from  $\alpha=0$  ( $\beta=0.2$ ) to  $\alpha=0.8$  ( $\beta=1$ ). Note that the convergence is slower if the overlap is in the center. As the overlap moves towards the

boundary convergence gets faster and faster, until instantaneous convergence is obtained if one subdomain spans the whole domain.

## 5. Superlinear Convergence on Bounded Time Intervals

We consider now bounded time intervals,  $t \in [0, T)$ ,  $T < \infty$ . with the usual infinity norm for functions in  $L^{\infty}([0, T); \mathbb{R})$ ,

$$||f(\cdot)||_T := \sup_{0 < t < T} |f(t)|.$$

We are generalizing ideas introduced by Giladi and Keller in [10] for linear parabolic problems. A reformulation of their analysis in terms of Maximum Principles permits the extension of their results to reaction diffusion equations. The following Lemma establishes superlinear convergence of the overlapping Schwarz waveform relaxation algorithm on the interfaces.

**Lemma 5.1.** Suppose that the derivative of f in (3.1) is uniformly bounded from above, f'(u) < a for all  $u \in IR$ . Then the error in the iteration (3.6), (3.7) decays superlinearly on the interfaces  $x = \alpha L$  and  $x = \beta L$ . Specifically

$$||d^{2k}(\alpha L, \cdot)||_T \leq \max(e^{aT}, 1) \operatorname{erfc}(\frac{k(\beta - \alpha)L}{\sqrt{c^2T}}) ||d^0(\alpha L, \cdot)||_T$$
(5.1)

$$||e^{2k}(\beta L,\cdot)||_T \leq \max(e^{aT},1)erfc(\frac{k(\beta-\alpha)L}{\sqrt{c^2T}})||e^0(\beta L,\cdot)||_T.$$
 (5.2)

*Proof* Consider the differential equation on the quarter plane,

Its solution is shown in Cannon [5] to be

$$\tilde{d}^{k+2} = \int_0^t K_x(\beta L - x, t - \tau) e^{a(t-\tau)} |e^{k+1}(\beta L, \tau)| d\tau, \tag{5.4}$$

where the kernel  $K_x(x,t)$  is given by

$$K_x(x,t) = \frac{x}{2\sqrt{\pi}ct^{3/2}}e^{-\frac{x^2}{4c^2t}}. (5.5)$$

Thus  $\tilde{d}^{k+2}$  is non-negative. Consider the difference  $w:=\tilde{d}^{k+2}-d^{k+2}$  which satisfies the differential equation

$$\frac{\partial w}{\partial t} = c^2 \frac{\partial^2 w}{\partial x^2} + a\tilde{d}^{k+2} - f'(\eta^{k+2})d^{k+2}$$
$$= c^2 \frac{\partial^2 w}{\partial x^2} + (a - f'(\eta^{k+2}))\tilde{d}^{k+2} + f'(\eta^{k+2})w.$$

Since a is an upper bound on the derivative of f and  $\tilde{d}^{k+2}$  is non-negative the term  $(a-f'(\eta^{k+2}))\tilde{d}^{k+2}$  is non-negative and thus w satisfies the differential inequalities

By the Positivity Lemma  $w=\tilde{d}^{k+2}-d^{k+2}\geq 0$ . A similar result holds for the sum  $\tilde{w}:=\tilde{d}^{k+2}+d^{k+2}\geq 0$  and hence the modulus of  $d^{k+2}(x,t)$  can be bounded by

$$|d^{k+2}(x,t)| \le \tilde{d}^{k+2} = \int_0^t K_x(\beta L - x, t - \tau) e^{a(t-\tau)} |e^{k+1}(\beta L, \tau)| d\tau.$$
 (5.7)

By a similar argument the modulus of  $e^{k+1}(x,t)$  can be bounded by

$$|e^{k+1}(x,t)| \le \int_0^t K_x(x-\alpha L, t-\tau)e^{a(t-\tau)}|d^k(\alpha L, \tau)|d\tau,$$
 (5.8)

Evaluating (5.8) at  $\beta L$  and inserting it into (5.7) one obtains

$$|d^{k+2}(x,t)| \le \int_0^t K_x(\beta L - x, t - \tau) e^{a(t-\tau)} \int_0^\tau K_x((\beta - \alpha)L, \tau - s) e^{a(\tau - s)} |d^k(\alpha L, s)| ds d\tau.$$
(5.9)

By induction

$$|d^{2k}(\alpha L, t)| \leq \int_{0}^{t} K_{x}((\beta - \alpha)L, t - s_{1})e^{a(t - s_{1})} \cdots \int_{0}^{s_{2k-1}} K_{x}((\beta - \alpha)L, s_{2k-1} - s_{2k})e^{a(s_{2k-1} - s_{2k})}|d^{0}(\alpha L, s_{2k})|ds_{2k} \cdots ds_{1}.$$
(5.10)

First note that the exponential terms can be combined, because

$$e^{a(t-s_1)}e^{a(s_1-s_2)}\dots e^{a(s_{2k-1}-s_{2k})}=e^{a(t-s_{2k})}$$

Hence one can take the supremum of  $e^{a(t-s_{2k})}$  and  $|d^0(\alpha L, s_{2k})|$  out of the integral,

$$|d^{2k}(\alpha L, t)| \leq ||d^{0}(\alpha L, \cdot)||_{t} \max(e^{at}, 1) \int_{0}^{t} K_{x}((\beta - \alpha)L, t - s_{1}) \cdots \int_{0}^{s_{2k-1}} K_{x}((\beta - \alpha)L, s_{2k-1} - s_{2k}) ds_{2k} \cdots ds_{1}.$$

$$(5.11)$$

To unfold the convolutions, note that the Laplace transform of a convolution is the product of the Laplace transformed kernels. In our case the Laplace transform of the kernel is (Abramowitz [1])

$$\int_0^\infty e^{st} K_x((\beta - \alpha)L, t) dt = e^{-\frac{(\beta - \alpha)L}{2c}\sqrt{s}}$$

and thus the 2k-fold convolution is the product of identical exponentials in the Laplace transformed domain,

$$e^{-\frac{2k(\beta-\alpha)L}{2c}\sqrt{s}}$$

Backtransforming this expression, one finds the bound

$$|d^{2k}(\alpha L, t)| \le ||d^0(\alpha L, \cdot)||_t \max(e^{at}, 1) \int_0^t K_x(2k(\beta - \alpha)L, t - \tau) d\tau.$$
 (5.12)

Performing the variable transform

$$y := \frac{k(\beta - \alpha)L}{\sqrt{c^2(t - \tau)}}$$

in the integration leads to

$$|d^{2k}(\alpha L, t)| \leq \max(e^{at}, 1)\operatorname{erfc}(\frac{k(\beta - \alpha)L}{\sqrt{c^2t}})||d^0(\alpha L, \cdot)||_t$$

Noting that the expression on the right is nondecreasing in t inequality (5.1) follows. Inequality (5.2) is obtained similarly.

Defining for any function g(x,t) in  $L^{\infty}([a,b],L^{\infty})$  the norm

$$|||g(\cdot,\cdot)|||_T := \sup_{a < x < b} ||g(x,\cdot)||_T$$

one obtains

**Theorem 5.1. (Superlinear Convergence)** Assume that f' in (3.1) is uniformly bounded from above by an arbitrary constant a. Then the overlapping Schwarz waveform relaxation algorithm for the reaction diffusion equation (3.1) with two subdomains converges superlinearly for any initial guess at a rate depending on the size of the overlap, the length of the time interval and the diffusion coefficient. Specifically

$$|||d^{2k+1}(\cdot,\cdot)|||_T \le \max(e^{2aT},1)erfc(\frac{k(\beta-\alpha)L}{\sqrt{c^2T}})||e^0(\beta L,\cdot)||_T$$
 (5.13)

$$|||e^{2k+1}(\cdot,\cdot)|||_T \le \max(e^{2aT},1)erfc(\frac{k(\beta-\alpha)L}{\sqrt{c^2T}})||d^0(\alpha L,\cdot)||_T.$$
 (5.14)

*Proof* From inequality (5.7) in Lemma 5.1. one gets

$$|d^{2k+1}(x,t)| \le ||e^{2k}(\beta L,\cdot)||_T \int_0^T K_x(\beta L - x, T - \tau)e^{a(t-\tau)}d\tau.$$

Taking the maximum of the exponential out of the integral and noting that the remaining integral is bounded by unity, one gets.

$$|d^{2k+1}(x,t)| \le \max(e^{aT},1)||e^{2k}(\beta L,\cdot)||_T.$$

Now application of Lemma 5.1. leads to the desired result. The second inequality is obtained similarly.

**Remark:** It is interesting to note that this superlinear convergence rate is faster than the traditional superlinear convergence rate, which is of the form  $(CT)^k/k!$  for waveform relaxation algorithms with matrix splittings, since asymptotically

$$\operatorname{erfc}(Ck) \sim \frac{1}{\sqrt{\pi}Ck} e^{-k^2C^2}$$
 whereas  $\frac{C^k}{k!} \sim \frac{1}{\sqrt{2\pi k}} e^{-k \ln k + (1+\ln C)k}$ .

#### 6. Variable Diffusion Coefficient

To obtain explicit convergence rates we need to bound the solution of the partial differential equation with variable coefficients with the solution of a constant coefficient equation. Then the above analysis can be applied. Such comparison results are obtained in the following subsections.

## 6.1. Steady State Upper Bound

Consider the differential equation with variable coefficients,

where a(x,t) is a function bounded from below,  $a(x,t) \geq C$  for some constant C and  $c_1 \leq c^2(x,t) \leq c_2$  for strictly positive constants  $0 < c_1 \leq c_2$  for all  $x \in (0,L)$  and  $t \in (0,\infty)$  and compare it with the constant coefficient steady state equation

$$0 = \hat{c}^2 \frac{\partial^2 v}{\partial x^2} + \hat{a}v \qquad 0 < x < \beta L$$

$$v(0) = 0$$

$$v(\beta L) = ||g(\cdot)||_{\infty}$$

$$(6.2)$$

# **Lemma 6.1.** *If*

$$\hat{c}^2 = \sup_{x,t} c^2(x,t) , \quad \hat{a} \ge \hat{c}^2 \frac{a(x,t)}{c^2(x,t)}, \quad 0 \le x \le \beta L, \ t > 0$$
 (6.3)

and

$$\hat{a} \le \left(\frac{\hat{c}\pi}{\beta L}\right)^2 \tag{6.4}$$

then v(x) is a bound on |u(x,t)|,  $v(x) \ge |u(x,t)|$ ,  $0 \le x \le \beta L$ , t > 0.

*Proof* Define the difference w(x,t) := v(x) - u(x,t). Then w satisfies

$$\frac{\partial w}{\partial t} = \hat{c}^2 \frac{\partial^2 v}{\partial x^2} - c^2(x, t) \frac{\partial^2 u}{\partial x^2} + \hat{a}v - a(x, t)u$$

$$= (\hat{c}^2 - c^2(x, t)) \frac{\partial^2 v}{\partial x^2} + c^2(x, t) \frac{\partial^2 w}{\partial x^2} + (\hat{a} - a(x, t))v + a(x, t)w.$$

So if we can show that

$$F(x,t) := (\hat{c}^2 - c^2(x,t)) \frac{\partial^2 v}{\partial x^2} + (\hat{a} - a(x,t))v \ge 0$$

then by the Positivity Lemma  $w(x,t) \ge 0$  and we are done. Using the differential equation (6.2) we have

$$\frac{\partial^2 v}{\partial x^2} = -\frac{\hat{a}}{\hat{c}^2} v$$

and thus

$$F(x,t) = \left(-\frac{\hat{a}(\hat{c}^2 - c^2(x,t))}{\hat{c}^2} + \hat{a} - a(x,t)\right)v.$$

Now note that  $v \ge 0$  with condition (6.4). So the second factor in F(x, t) is non-negative, and the first one becomes non-negative using the conditions (6.3), since

$$\frac{-\hat{a}(\hat{c}^2 - c^2(x,t)) + \hat{a}\hat{c}^2 - a(x,t)\hat{c}^2}{\hat{c}^2} = \frac{\hat{a}c^2(x,t) - a(x,t)\hat{c}^2}{\hat{c}^2} \ge 0,$$

which concludes the proof.

Using this lemma to construct an upper bound, the linear convergence results can be extended to a variable diffusion coefficient.

# 6.2. Superlinear Upper Bound

Consider the differential equation with variable coefficients,

$$\frac{\partial u}{\partial t} = c^{2}(x,t)\frac{\partial^{2} u}{\partial x^{2}} + a(x,t)u \qquad x < \beta L, \ 0 < t < T 
 u(\beta L,t) = g(t) \qquad 0 < t < T 
 u(x,0) = 0 \qquad x \le \beta L,$$
(6.5)

where a(x,t) is a function bounded from below,  $a(x,t) \geq C$  for some constant C and  $c_1 \leq c^2(x,t) \leq c_2$  for strictly positive constants  $0 < c_1 \leq c_2$  for all  $x \in (0,L)$  and  $t \in (0,T]$  and compare it with the constant coefficient equation

$$\frac{\partial v}{\partial t} = \hat{c}^2 \frac{\partial^2 v}{\partial x^2} + \hat{a}v \qquad x < \beta L, \ 0 < t < T 
v(\beta L, t) = ||g(\cdot)||_t \qquad 0 < t < T 
v(x, 0) = 0 \qquad x \le \beta L.$$
(6.6)

Note that these are quarter plane problems.

# **Lemma 6.2.** *If*

$$\hat{c}^2 = \sup_{x,t} c^2(x,t) , \quad \hat{a} \ge \hat{c}^2 \frac{a(x,t)}{c^2(x,t)}, \quad 0 \le x \le \beta L, 0 < t < T$$
 (6.7)

then v(x, t) is an upper bound on u(x, t),

$$v(x,t) \ge |u(x,t)|, \quad x \le \beta L, \ 0 \le t \le T.$$

**Proof** Define the difference w(x,t) := v(x,t) - u(x,t). Then w satisfies

$$\begin{split} \frac{\partial w}{\partial t} &= \hat{c}^2 \frac{\partial^2 v}{\partial x^2} - c^2(x,t) \frac{\partial^2 u}{\partial x^2} + \hat{a}v - a(x,t)u \\ &= (\hat{c}^2 - c^2(x,t)) \frac{\partial^2 v}{\partial x^2} + c^2(x,t) \frac{\partial^2 w}{\partial x^2} + (\hat{a} - a(x,t))v + a(x,t)w. \end{split}$$

So if we can show that

$$F(x,t) := (\hat{c}^2 - c^2(x,t)) \frac{\partial^2 v}{\partial x^2} + (\hat{a} - a(x,t))v \ge 0$$

then by the Positivity Lemma  $w(x,t) \ge 0$  and we are done. Using the differential equation (6.6) we get

$$\frac{\partial^2 v}{\partial x^2} = \frac{1}{\hat{c}^2} \left( \frac{\partial v}{\partial t} - \hat{a}v \right)$$

and thus

$$F(x,t) = \frac{\hat{c}^2 - c^2(x,t)}{\hat{c}^2} \frac{\partial v}{\partial t} + \left( -\frac{\hat{a}(\hat{c}^2 - c^2(x,t))}{\hat{c}^2} + \hat{a} - a(x,t) \right) v.$$

Now  $\frac{\partial v}{\partial t} \geq 0$  on  $x = \beta L$  by the monotonicity of the boundary condition and at t = 0 since  $v(x,t) \geq 0$  by the Positivity Lemma. Since  $\frac{\partial v}{\partial t}$  satisfies a linear reaction diffusion equation as well, we have  $\frac{\partial v}{\partial t} \geq 0$  throughout the domain by the Positivity Lemma. Hence the first term in the sum is non-negative by the definition of  $\hat{c}^2$ . In the second term of the sum, the first factor is non-negative by the conditions of the Lemma and the second factor v(x,t) as well by the Positivity Lemma, which concludes the proof.

Using this lemma to construct an upper bound, the superlinear convergence results can be extended to variable coefficients.

#### 7. Numerical Experiments

We perform numerical experiments to measure the actual convergence rate of the overlapping Schwarz waveform relaxation algorithm and compare it with the theoretical bounds derived in the previous sections.

#### 7.1. Linear Example

Consider a linear example problem, for which the derived bounds are expected to be sharp,

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + au \qquad 0 < x < 1, \ 0 < t < T$$

$$u(0,t) = 0 \qquad 0 < t < T$$

$$u(1,t) = e^{-t} \qquad 0 < t < T$$

$$u(x,0) = x^2 \qquad 0 \le x \le 1.$$

$$(7.1)$$

First we choose a large time interval, T=4 to be in the linear convergence regime. To solve the partial differential equation, we discretize the Laplacian using centered finite differences and the backward Euler method in time on a grid with  $\Delta x=5\times 10^{-3}$  and  $\Delta t=4\times 10^{-3}$ . For the first experiment we choose the constant a=5 and split the domain  $\Omega=[0,1]\times[0,T)$  into the two subdomains  $\Omega_1=[0,\beta]\times[0,T)$  and  $\Omega_2=[\alpha,1]\times[0,T)$  for two different overlaps,  $(\alpha,\beta)\in\{(0.4,0.6),(0.45,0.55)\}$ . We call the grid point at the interface  $\beta L$  grid point b and measure the error in the infinity norm in time at this grid point. Figure 4 shows on the left the convergence of the algorithm at the grid point b for the two overlaps. The solid line is the predicted convergence rate according to Lemma 4.1. and the dashed line is the measured one. The iteration with the bigger overlap converges quicker as expected. The measured error displayed is the difference between the numerical solution on the whole domain and the solution obtained from the domain decomposition algorithm, and we used as an initial guess for the iteration the constant function  $v^0(x,t)=1$ . For the second experiment we fix the size of the overlap  $\alpha=0.4$  and  $\beta=0.6$  and vary the

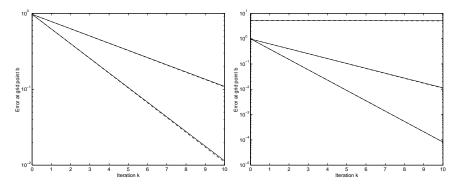


Figure 4. Theoretical and measured linear decay rate of the error for two different overlaps on the left and for three different values of a on the right

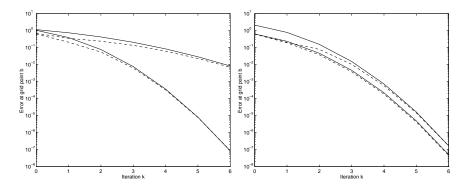


Figure 5. Theoretical and measured superlinear decay rate of the error for two different overlaps on the left and for two different values of a on the right

constant  $a \in \{-2, 5, \pi^2\}$ . The results are shown in Figure 4 on the right. Note how the iteration stagnates for  $a = \pi^2$ .

To test the superlinear convergence bounds, we choose a short time interval, T=0.1. Using the same numerical method as before on a grid with  $\Delta x=5\times 10^{-3}$  and  $\Delta t=1\times 10^{-4}$  we perform the above experiments again. Figure 5 shows on the left the superlinear convergence of the algorithm at the grid point b for the two overlaps and on the right the same overlap for two values of the constant  $a\in\{-2,12\}$ . The solid line is the predicted convergence rate according to Lemma 5.1. and the dashed line is the measured one. Note that the iteration converges in the superlinear regime even though the constant  $a>\pi^2$ . Furthermore one can see that the asymptotic convergence rate is not affected by the reaction term a, there is only a constant factor introduced for large a, as predicted by the analysis.

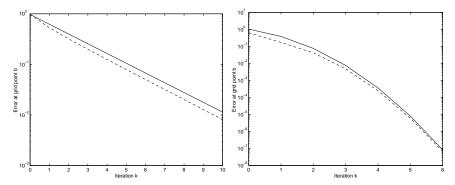


Figure 6. Theoretical and measured decay rates of the error for the nonlinear example problem

# 7.2. Nonlinear Example

Consider now a nonlinear example problem, namely

$$\begin{array}{rcl} \frac{\partial u}{\partial t} & = & \frac{\partial^2 u}{\partial x^2} + 5(u - u^3) & 0 < x < 1, \ 0 < t < T \\ u(0,t) & = & 0 & 0 < t < T \\ u(1,t) & = & e^{-t} & 0 < t < T \\ u(x,0) & = & x^2 & 0 \le x \le 1. \end{array} \tag{7.2}$$

We apply the same numerical method as in the linear case, except that we treat the nonlinear part explicitly in the backward Euler scheme. we split the domain with  $\alpha=0.4$  and  $\beta=0.6$ . Figure 6 shows on the left the convergence behavior for T=4 where the iteration is in the linear regime. The solid line is the predicted convergence rate according to Lemma 4.1. and the dashed line is the measured one. On the right, Figure 6 shows the superlinear convergence behavior of the algorithm for T=0.1. As before the solid line denotes the predicted convergence rate according to Lemma 5.1. and the dashed line is the measured one.

## 8. Generalization and Future Directions

We first want to show how sharper estimates can be obtained than the ones stemming from the global assumptions on the growth of the reaction function f. Both the linear convergence Theorem 4.1. and the superlinear convergence Theorem 5.1. establish a uniform contraction in a ball  $B \subset L^{\infty}([a,b],L^{\infty})$ . The radius of the ball depends on the growth rate of the reaction function, the quality of the initial guess and in the superlinear case on the length of the time interval. Since all the iterates remain in the ball B, the constant a in the convergence rates stemming from the global boundedness assumption on the derivative of the reaction function can be sharpened using the local estimate  $f'(u) \leq a$  for  $u \in B$  and Theorems 4.1. and 5.1. still hold.

Second it is of interest to generalize the results for two subdomains to many subdomains to obtain an algorithm which can be run in parallel. The linear convergence result in Theorem 4.1. can be generalized in the same way as the result for the heat equation

was generalized in [8]. The resulting convergence rate however will depend on the number of subdomains as in the heat equation case, and the convergence will slow down as one increases the number of subdomains, because information from the boundary of the whole domain has to propagate into the interior across subdomains, taking one iteration to cross each subdomain. This is because the steady state case is limiting the convergence rate on unbounded time intervals. This is different when the superlinear convergence result in Theorem 5.1. is generalized to many subdomains. Here information is propagated from the initial condition, to which every subdomain is directly connected. Hence the convergence rate will not depend on the number of subdomains. This can be seen directly from the local decay properties of the kernel functions in the proof of Theorem 5.1. and is analogous to the heat equation case investigated in [7].

Finally for applications results in higher spatial dimesions would be needed. The main tool in the convergence analysis of the one dimensional case is the Positivity Lemma 2.1.. This Lemma holds in higher dimensions as well [22]. In the heat equation case, the one dimensional results in [8] have been generalized to n dimensions in [9] by first using the maximum principle in higher dimensions and then reducing the estimates to the one dimensional case. Such an approach is currently pursued in the reaction diffusion case.

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