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## Fractional-Splitting and Domain-Decomposition Methods for Parabolic Problems and Applications

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## Abstract

In this paper we consider the first order fractional splitting method to solve decomposed complex equations with multi-physical processes for applications in porous media and phase-transitions. The first order fractional splitting method is also considered as basic solution for the overlapping Schwarz-Waveform-Relaxation method for an overlapped subdomains. The accuracy and the efficiency of the methods are investigated through the solution of different model problems of scalar, coupling and decoupling systems of convection reaction diffusion equation.

## 1 Introduction

We motivate our studying on complex models with coupled processes, e.g. transport and reaction-equations with nonlinear parameters. The ideas for these models came from the background of the simulation of heat transport in engineering apparatus, e.g. crystal-growth, cf. [12], or the simulation of chemical reaction and transport, e.g. in bio-remediation or waste disposals, cf. [10]. In the past many software-tools have been developed for multi-dimensional and multi-physical problems, e.g. multi-dimensional transport-reaction based on different PDE and ODE solvers. In the future a coupling between various software-tools with different solver methods will be of interest and could be done with the fractional splitting method.

We consider the overlapped domain decomposition method, such as overlapping Schwarz wave form relaxation, cf. [9] and [13], using fractional splitting as the basic solver over the overlapped subdomains.

The outline of the paper is as follows. For our mathematical model we describe the convection-diffusion-reaction equation in section 2. The Fractional-Splitting method is introduced in section 3. For the overlapping Schwarz-Waveform-Relaxation method we derive the error-analysis for the scalar and systems of equations (coupled or decoupled systems) and presented the results in section 4. In section 5 we present the numerical results from the solution to selective model problems. We end the article in section 6 with conclusion and comments.

## 2 Mathematical Model

The motivation for the study presented below is coming from a computational simulation of heat-transfer [12] and convection-diffusion-reaction-equations [10].

The mathematical equations are given by

$$\partial_t R u + \nabla \cdot (\mathbf{v}u - D\nabla u) = f(x, t, u(x, t)) , \text{ in } \Omega \times (0, T) , \quad (2.1)$$

$$u(x, 0) = u_0(x) , \text{ (Initial-Condition) ,} \quad (2.2)$$

$$u(x, t) = u_1(x, t) , \text{ on } \partial\Omega \times (0, T) , \text{ (Dirichlet-Boundary-Condition) ,} \quad (2.3)$$

The unknown  $u = u(x, t)$  is considered in  $\Omega \times (0, T) \subset \mathbb{R}^d \times \mathbb{R}$ , the space-dimension is given by  $d$ . The parameter  $R \in \mathbb{R}^+$  is a constant and named as specific heat or retardation factor. The parameters  $u_0(x), u_1(x, t) \in \mathbb{R}^+$  are functions and used as initial- and boundary-parameter respectively.  $D$  is the thermal conductivity tensor or Scheidegger diffusion-dispersion tensor and  $\mathbf{v}$  is the velocity. Further  $f(x, t, u)$  is a possible nonlinear function, and one could choose it for the following applications :

$$f(x, t, u) = u^p , \text{ with } p > 0 , \text{ chemical-reaction ,} \quad (2.4)$$

$$f(x, t, u) = \frac{u}{1-u} , \text{ bio-remediation ,} \quad (2.5)$$

$$f(x, t, u) = \tilde{f}(x, t) , \text{ heat-induction .} \quad (2.6)$$

The aim of this paper is to present a new method based on a mixed discretization method with Fractional-Splitting and Domain decomposition methods for an effective solving of strong coupled parabolic differential equations.

In the next section we discuss the fractional splitting-methods for solving our equations.

## 3 Fractional-Splitting Methods

### 3.1 Splitting methods of first order for linear equations

First we describe the simplest operator-splitting, which is called *sequential operator splitting* for the following system of ordinary linear differential equations:

$$\partial_t u(t) = A u(t) + B u(t) , \text{ in } \Omega \times [t^n, t^{n+1}] , \quad (3.1)$$

where the initial-conditions are  $u^n = u(t^n)$ . The operators  $A$  and  $B$  are spatially discretised operators, e.g. they correspond to the discretised in space convection and diffusion operators (matrices). Hence, they can be considered as bounded operators.

The sequential operator-splitting method is introduced as a method which solve the two sub-problems sequentially, where the different sub-problems are connected via the initial conditions. This means that one replaces the original problem (3.1) with the sub-problems

$$\begin{aligned} \frac{\partial u^*(t)}{\partial t} &= A u^*(t) , \quad \text{with } u^*(t^n) = u^n , \\ \frac{\partial u^{**}(t)}{\partial t} &= B u^{**}(t) , \quad \text{with } u^{**}(t^n) = u^*(t^{n+1}) , \end{aligned} \quad (3.2)$$

where the splitting time-step is defined as  $\tau_n = t^{n+1} - t^n$ . The approximated split solution is defined as  $u^{n+1} = u^{**}(t^{n+1})$ .

Clearly, the change of the original problems with the sub-problems usually results some error, called *splitting error*. Obviously, the splitting error of the sequential operator splitting method can be derived as follows (cf. e.g. [10])

$$\begin{aligned} \rho_n &= \frac{1}{\tau} (\exp(\tau_n(A+B)) - \exp(\tau_n B) \exp(\tau_n A)) u(t^n) \\ &= \frac{1}{2} \tau_n [A, B] u(t^n) + O(\tau^2). \end{aligned} \tag{3.3}$$

where  $[A, B] := AB - BA$  is the commutator of  $A$  and  $B$ . Consequently, the splitting error is  $O(\tau_n)$  when the operators  $A$  and  $B$  do not commute, otherwise the method is exact. Hence, by definition, the sequential operator splitting is called *first order splitting method*.

Now we introduce the domain-decomposition methods as next idea for splitting methods to decompose complex domains and solve them effectively in an adaptive method.

## 4 Overlapping Schwarz wave form relaxation for the solution to convection-diffusion-reaction equation

The first known method for solving partial differential equation over overlapped domains is the Schwarz method due to [23] in 1869. In the last years massive parallel computers are used for simulating complex problems, therefore the method has regained its popularity, because it can be implemented as a parallel method.

Further techniques have been developed for the general cases when the domains are overlapped and non overlapped. For each class of methods there are some interesting features and both share same concepts which is how to define the interface boundary conditions over the overlapped or along the non overlapped subdomains. The general solution methods over the whole subdomains together with the interface boundary conditions estimations are either iterative or non iterative methods.

For the non overlapping subdomains the values at the interfaces are predicted by using an explicit scheme and the problem is solved over each subdomain independently. This type of method is of non iterative type but it has a drawback regarding the stability condition for the interface prediction by the explicit method and the solution by the implicit scheme or any other unconditional stable finite difference scheme [24].

For the overlapping subdomains the determination of the interface boundary condition is defined by using predictor corrector type of method. The predictor will

provide an estimation of the boundary condition while the correction is performed from the updated solution over the subdomains. These types of the algorithms are iterative types with the advantage of stabilising the iterative values at the interface through the overlapping. The overlapping is used as a relaxation-method of the solution in the interface region.

In this work we will consider the overlapping type of domain decomposition method for solving the studied models of constant coefficients, decoupled and coupled systems solved by using the first order operator splitting algorithm with a backward Euler difference scheme. The most recent method in this field is the overlapping Schwarz waveform relaxation scheme, see [9] and [13].

Overlapping Schwarz waveform relaxation is the name for a combination of two standard algorithms, the Schwarz alternating method and the wave form relaxation algorithm to solve evolution problems in parallel. The method is defined by partitioning the spatial domain into overlapping sub-domains, as in the classical Schwarz method. However on sub-domains, time dependent problems are solved in the iteration and thus the algorithm is also of waveform relaxation type. Further more, the problem is solved using the operator splitting of first order over each sub-domain. The overlapping Schwarz waveform relaxation are introduced in [13] and independently in [9] as a solver method of evolution problems in a parallel environment with slow communication links. The idea is to solve over several time steps before communicating information to the neighboring sub-domains and updating the calculated interface boundary conditions for the overlapped domains.

Two forms of convergence behavior have been observed for the convergence of the overlapping Schwarz wave form relaxation method. The convergence behavior states linear convergence on bounded time domain and super linear convergence over short time domain [9].

This algorithm stands in contrast to the classical approach in domain decomposition for evolution problems, where time is first discretized uniformly using an implicit discretization and then at each time step a problem in space only is solved using domain decomposition, see for example [18] and [2, 3]. Further more, in this work the operator splitting method will be considered by using Crank-Nicolson (CN) or an implicit Euler-method for the time-discretisation. The main advantage in considering the overlapping Schwarz wave form relaxation method is the flexibility that one can solve over each sub-domain with different time steps and different spatial steps in the whole time-interval. In this section we will consider the Schwarz wave form relaxation to solve scalar, and systems of convection-reaction-diffusion equations. For the systems of convection-reaction-diffusion equations we study the weak coupled case, i.e. two equations coupled by the reaction-terms.

In this work the studied model problems are defined over unbounded time interval, or long time interval. We will show how the convergence of the iterated solutions are of linear convergence behavior.

## 4.1 Overlapping Schwarz wave form relaxation for the scalar convection-diffusion-reaction equation

We consider the convection-diffusion-reaction equation, given by

$$Ru_t = Du_{xx} - \nu u_x - \lambda u, \quad (4.1)$$

defined on the domain  $\Omega = [0, L]$  for  $T = [t_0, t_{\text{end}}]$ , where  $L, t_{\text{end}} \in \mathbb{R}^+$ , and  $R, D, \nu, \lambda \in \mathbb{R}^+$  and bounded, with the following initial and boundary conditions

$$u(0, t) = f_1(t), \quad u(L, t) = f_2(t), \quad u(x, t_0) = u_0(x).$$

We have the following theorem, see [5] or [19], that shows the existency, uniqueness and regularity of the solution to the concerned boundary value problem for (4.1).

**Theorem 4.1.** *For any  $L_1, L_2 \in [0, L]$  with  $L_1 < L_2$  and any continuous functions  $f_1, f_2 : [t_0, t_{\text{end}}] \rightarrow \mathbb{R}$  and any  $u_0 : [L_1, L_2] \rightarrow \mathbb{R}$  which satisfy the compatibility conditions  $u_0(L_1) = f_1(t_0)$  and  $u_0(L_2) = f_2(t_0)$  the boundary value-problem (4.1) and  $u(L_1, t) = f_1(t)$ ,  $u(L_2, t) = f_2(t)$ ,  $u(x, t_0) = u_0(x)$  has a unique solution. The solution  $u$  lies in  $C^{2,1}([L_1, L_2], [t_0, t_{\text{end}}])$ , that means  $u(\cdot, t) \in C^2$  and  $u(x, \cdot) \in C^1$ .*

To solve the model problem using overlapping Schwarz wave form relaxation method, we subdivide the domain  $\Omega$  in two overlapping sub-domains  $\Omega_1 = [0, L_2]$  and  $\Omega_2 = [L_1, L]$ , where  $L_1 < L_2$  and  $\Omega_1 \cap \Omega_2 = [L_1, L_2]$  is the overlapping region for  $\Omega_1$  and  $\Omega_2$ .

To start the wave form relaxation algorithm we firstly consider the solution to the model problem (4.1) over  $\Omega_1$  and  $\Omega_2$  as follows

$$\begin{aligned} Rv_t &= Dv_{xx} - \nu v_x - \lambda v \text{ over } \Omega_1, \quad t \in [t_0, t_{\text{end}}] \\ v(0, t) &= f_1(t), \quad t \in [t_0, t_{\text{end}}] \\ v(L_2, t) &= w(L_2, t), \quad t \in [t_0, t_{\text{end}}] \\ v(x, t_0) &= u_0(x), \quad x \in \Omega_1, \end{aligned} \quad (4.2)$$

$$\begin{aligned} Rv_t &= Dw_{xx} - \nu w_x - \lambda w \text{ over } \Omega_2, \quad t \in [t_0, t_{\text{end}}] \\ w(L_1, t) &= v(L_1, t), \quad t \in [t_0, t_{\text{end}}] \\ w(L, t) &= f_2(t), \quad t \in [t_0, t_{\text{end}}] \\ w(x, t_0) &= u_0(x), \quad x \in \Omega_2, \end{aligned} \quad (4.3)$$

where  $v(x, t) = u(x, t)|_{\Omega_1}$  and  $w(x, t) = u(x, t)|_{\Omega_2}$ . For the uniqueness and existence we apply theorem 4.1. We fulfill the criterias by the possitivity and boundedness of the parameters  $R, D, \nu$  and  $\lambda$  and also of the intial- and boundary-conditions.

Therefore we will obtain the overlapping Schwarz wave form relaxation from solving (4.2) and (4.3) over the whole time domain for each iteration, and then updating the interior boundary conditions  $v(L_2, t)$  and  $w(L_1, t)$ . The algorithm is given by

$$\begin{aligned} Rv_t^{k+1} &= Dv_{xx}^{k+1} - \nu v_x^{k+1} - \lambda v^{k+1} \text{ over } \Omega_1, \quad t \in [t_0, t_{\text{end}}] \\ v^{k+1}(0, t) &= f_1(t), \quad t \in [t_0, t_{\text{end}}] \\ v^{k+1}(L_2, t) &= \begin{cases} w^k(L_2, t) & \text{for } k > 0 \\ u_0(L_2) & \text{for } k = 0 \end{cases}, \quad t \in [t_0, t_{\text{end}}] \\ v^{k+1}(x, t_0) &= u_0(x), \quad x \in \Omega_1, \end{aligned} \quad (4.4)$$

$$\begin{aligned}
Rw_t^{k+1} &= Dw_{xx}^{k+1} - \nu w_x^{k+1} - \lambda w^{k+1} \text{ over } \Omega_2, \quad t \in [t_0, t_{\text{end}}) \\
w^{k+1}(L_1, t) &= \begin{cases} v^k(L_1, t) & \text{for } k > 0 \\ u_0(L_1) & \text{for } k = 0 \end{cases}, \quad t \in [t_0, t_{\text{end}}) \\
w^{k+1}(L, t) &= f_2(t), \quad t \in [t_0, t_{\text{end}}) \\
w^{k+1}(x, t_0) &= u_0(x), \quad x \in \Omega_2.
\end{aligned} \tag{4.5}$$

For the uniqueness and existence of the partial equations (4.4) and (4.5) we apply theorem 4.1.

We are interested in estimating the decay of the error of the solution over the overlapping subdomains by the overlapping Schwarz wave form relaxation method.

Let us assume  $e(x, t) = u(x, t) - v(x, t)$  and  $d(x, t) = u(x, t) - w(x, t)$  is the error of (4.4) over  $\Omega_1$  and (4.5) over  $\Omega_2$  respectively. The corresponding differential equations satisfied by  $e(x, t)$  and  $d(x, t)$  are given by

$$\begin{aligned}
Re_t^{k+1} &= De_{xx}^{k+1} - \nu e_x^{k+1} - \lambda e^{k+1} \text{ over } \Omega_1, \quad t \in [t_0, t_{\text{end}}) \\
e^{k+1}(0, t) &= 0, \quad t \in [t_0, t_{\text{end}}) \\
e^{k+1}(L_2, t) &= d^k(L_2, t), \quad t \in [t_0, t_{\text{end}}) \\
e^{k+1}(x, t_0) &= 0 \quad x \in \Omega_1,
\end{aligned} \tag{4.6}$$

$$\begin{aligned}
Rd_t^{k+1} &= Dd_{xx}^{k+1} - \nu d_x^{k+1} - \lambda d^{k+1} \text{ over } \Omega_2, \quad t \in [t_0, t_{\text{end}}) \\
d^{k+1}(L_1, t) &= e^k(L_1, t), \quad t \in [t_0, t_{\text{end}}) \\
d^{k+1}(L, t) &= 0, \quad t \in [t_0, t_{\text{end}}) \\
d^{k+1}(x, t_0) &= 0, \quad x \in \Omega_2.
\end{aligned} \tag{4.7}$$

For  $\tilde{\Omega} \subset \Omega$  and  $\tilde{L} \in \tilde{\Omega}$  we define for bounded functions  $h : \tilde{\Omega} \times [t_0, t_{\text{end}}) \rightarrow \mathbf{R}$  the following supremums norm

$$\|h(\tilde{L}, \cdot)\|_\infty := \sup_{t \in [t_0, t_{\text{end}})} |h(\tilde{L}, t)|.$$

For the convergence and error bound of  $e^{k+1}$  and  $d^{k+1}$  are presented by the following theorem

**Theorem 4.2.** *Let  $\{e^{k+1}\}$  and  $\{d^{k+1}\}$  be the sequences of errors from the solution to the subproblems (4.2) and (4.3) by Schwarz wave form relaxation over  $\Omega_1$  and  $\Omega_2$ , respectively, then*

$$|e^{k+2}(x, t)| \leq \gamma \|e^k(L_1, \cdot)\|_\infty, \quad \forall x \in \Omega_1,$$

and

$$|d^{k+2}(x, t)| \leq \gamma \|d^k(L_2, \cdot)\|_\infty, \quad \forall x \in \Omega_2,$$

for all  $t \in [t_0, t_{\text{end}})$ , where

$$\gamma = \frac{\sinh(\beta L_1) \sinh(\beta(L - L_2))}{\sinh(\beta L_2) \sinh(\beta(L - L_1))}, \quad \text{with } \beta = \frac{\sqrt{\nu^2 + 4D\lambda}}{2D}.$$



It holds for all  $(x, t) \in (\Omega_1 \times [t_0, t_{\text{end}}])$

$$|e^{2n+1}(x, t)| \leq \gamma_{\max,1}^n \|e^1(L_1, \cdot)\|_\infty ,$$

where

$$\gamma_{\max,1} = \max_{x \in [0, L_2]} \left( \exp(x - L_1) \frac{\sinh(\beta x) \sinh(\beta(L - L_2))}{\sinh(\beta L_2) \sinh(\beta(L - L_1))} \right) .$$

It holds for all  $(x, t) \in (\Omega_2 \times [t_0, t_{\text{end}}])$

$$|d^{2n+1}(x, t)| \leq \gamma_{\max,2}^n \|d^1(L_2, \cdot)\|_\infty ,$$

where

$$\gamma_{\max,2} = \max_{x \in [L_1, L]} \left( \exp(x - L_2) \frac{\sinh(\beta L_1) \sinh(\beta(L_2 - L))}{\sinh(\beta x) \sinh(\beta(L_1 - L))} \right) .$$

The errors  $e^0$  and  $d^0$  are bounded as :

$$\|e^0(L_1, \cdot)\|_\infty \leq \max_{t \in [t_0, t_{\text{end}}]} \{ \max\{|f_1(t)|, |f_2(t)|, |u_0(L_1)|\} \} ,$$

and

$$\|d^0(L_2, \cdot)\|_\infty \leq \max_{t \in [t_0, t_{\text{end}}]} \{ \max\{|f_1(t)|, |f_2(t)|, |u_0(L_2)|\} \} ,$$

*Proof.* To estimate the error  $e^{k+1}$  and  $d^{k+1}$ , consider the following differential equations defining  $\hat{e}^{k+1}$  and  $\hat{d}^{k+1}$

$$\begin{aligned} \hat{e}_t^{k+1} &= D \hat{e}_{xx}^{k+1} - \nu \hat{e}_x^{k+1} - \lambda \hat{e}^{k+1} \text{ over } \Omega_1 , \quad t \in [t_0, t_{\text{end}}] , \\ \hat{e}^{k+1}(0, t) &= 0 , \quad t \in [t_0, t_{\text{end}}] , \\ \hat{e}^{k+1}(L_2, t) &= \|d^k(L_2, \cdot)\|_\infty , \quad t \in [t_0, t_{\text{end}}] , \\ \hat{e}^{k+1}(x, t_0) &= e^{(x-L_2)\alpha} \frac{\sinh(\beta x)}{\sinh(\beta L_2)} \|d^k(L_2, t)\|_\infty , \quad x \in \Omega_1 , \end{aligned} \tag{4.8}$$

and

$$\begin{aligned} \hat{d}_t^{k+1} &= D \hat{d}_{xx}^{k+1} - \nu \hat{d}_x^{k+1} - \lambda \hat{d}^{k+1} \text{ over } \Omega_2 , \quad t \in [t_0, t_{\text{end}}] , \\ \hat{d}^{k+1}(L_1, t) &= \|e^k(L_1, t)\|_\infty , \quad t \in [t_0, t_{\text{end}}] , \\ \hat{d}^{k+1}(L, t) &= 0 , \quad t \in [t_0, t_{\text{end}}] , \\ \hat{d}^{k+1}(x, t_0) &= e^{(x-L_1)\alpha} \frac{\sinh \beta(L-x)}{\sinh \beta(L-L_1)} \|e^k(L_1, t)\|_\infty , \quad x \in \Omega_2 , \end{aligned} \tag{4.9}$$

where  $\alpha = \frac{\nu}{2D}$ .

The solution to (4.8) and (4.9) is the steady state solution given by

$$\hat{e}^{k+1}(x, t) = e^{(x-L_2)\alpha} \frac{\sinh(\beta x)}{\sinh(\beta L_2)} \|d^k(L_2, \cdot)\|_\infty ,$$

and

$$\hat{d}^{k+1}(x, t) = e^{(x-L_1)\alpha} \frac{\sinh \beta(L-x)}{\sinh \beta(L-L_1)} \|e^k(L_1, \cdot)\|_\infty ,$$

respectively.

For the error between the steady state and time-dependent solution that is defined by  $E(x, t) = \hat{e}^{k+1} - e^{k+1}$ , it holds that

$$\begin{aligned} RE_t - DE_{xx} + \nu E_x + \lambda E &\geq 0, \text{ over } \Omega_1, \quad t \in [t_0, t_{\text{end}}), \\ E(0, t) &\geq 0, \quad t \in [t_0, t_{\text{end}}), \\ E(L_2, t) &\geq 0, \quad t \in [t_0, t_{\text{end}}), \\ E(x, t_0) &\geq 0, \quad x \in \Omega_1. \end{aligned} \quad (4.10)$$

Hence  $E(x, t)$  satisfies the positivity lemma by Pao (or the maximum principle theorem), see [19], therefore

$$E(x, t) \geq 0, \quad (4.11)$$

i.e.

$$|e^{k+1}(x, t)| \leq \hat{e}^{k+1}(x) = e^{(x-L_2)\alpha} \frac{\sinh(\beta x)}{\sinh(\beta L_2)} \|d^k(L_2, \cdot)\|_\infty, \quad (4.12)$$

for all  $(x, t) \in (\Omega_1 \times [t_0, t_{\text{end}}))$  and similarly one concludes that

$$|d^{k+1}(x, t)| \leq \hat{d}^{k+1}(x) = e^{(x-L_1)\alpha} \frac{\sinh \beta(x-L_1)}{\sinh \beta(L_1-L)} \|e^k(L_1, \cdot)\|_\infty ,$$

for all  $(x, t) \in (\Omega_2 \times [t_0, t_{\text{end}}))$ .

Therefore one gets the estimation with the supremums-norm :

We can conclude

$$|e^{k+1}(x, t)| \leq \|e^{k+1}(x, \cdot)\|_\infty ,$$

for all  $(x, t) \in (\Omega_1 \times [t_0, t_{\text{end}}))$ , and similar estimates for  $d^{k+1}$  can also be derived.

Then we conclude

$$\|e^{k+1}(x, \cdot)\|_\infty \leq e^{(x-L_2)\alpha} \frac{\sinh(\beta x)}{\sinh(\beta L_2)} \|d^k(L_2, \cdot)\|_\infty, \quad (4.13)$$

and

$$\|d^{k+1}(x, \cdot)\|_\infty \leq e^{(x-L_1)\alpha} \frac{\sinh \beta(x-L_1)}{\sinh \beta(L_1-L)} \|e^k(L_1, \cdot)\|_\infty. \quad (4.14)$$

Considering (4.14), evaluating  $d^k(x, t)$  for  $x = L_2$ , i.e.

$$\|d^k(L_2, \cdot)\|_\infty \leq e^{(L_2-L_1)\alpha} \frac{\sinh \beta(L_2-L)}{\sinh \beta(L_1-L)} \|e^{k-1}(L_1, \cdot)\|_\infty, \quad (4.15)$$

and substituting in (4.13), we conclude that

$$|e^{k+1}(x, t)| \leq e^{(x-L_2)\alpha} \frac{\sinh(\beta x)}{\sinh(\beta L_2)} e^{(L_2-L_1)\alpha} \frac{\sinh \beta(L_2 - L)}{\sinh \beta(L_1 - L)} \|e^{k-1}(L_1, \cdot)\|_\infty ,$$

and

$$e^{(x-L_2)\alpha} \sinh(\beta x) \leq e^{(L_1-L_2)\alpha} \sinh(\beta L_1) ,$$

consist for all  $(x, t) \in (\Omega_1, [t_0, t_{\text{end}}])$ .

One obtains

$$|e^{k+1}(L_1, t)| \leq e^{(L_1-L_2)\alpha} \frac{\sinh(\beta L_1)}{\sinh(\beta L_2)} e^{(L_2-L_1)\alpha} \frac{\sinh \beta(L_2 - L)}{\sinh \beta(L_1 - L)} \|e^{k-1}(L_1, \cdot)\|_\infty ,$$

for all  $(x, t) \in (\Omega_1, [t_0, t_{\text{end}}])$ .

And one gets the result

$$\|e^{k+2}(L_1, \cdot)\|_\infty \leq \frac{\sinh(\beta L_1)}{\sinh(\beta L_2)} \frac{\sinh \beta(L_2 - L)}{\sinh \beta(L_1 - L)} \|e^k(L_1, \cdot)\|_\infty .$$

Similarly for  $d^{k+1}(x, t)$  one concludes that

$$\|d^{k+2}(L_1, \cdot)\|_\infty \leq \frac{\sinh(\beta L_1)}{\sinh(\beta L_2)} \frac{\sinh \beta(L_2 - L)}{\sinh \beta(L_1 - L)} \|d^k(L_1, \cdot)\|_\infty .$$

□

Theorem 4.2 shows that the convergence of the overlapping Schwarz method depends on  $\gamma = \frac{\sinh(\beta L_1) \sinh \beta(L-L_2)}{\sinh(\beta L_2) \sinh \beta(L-L_1)}$ . Due to a large overlapping of the domains, we will have a relaxation and the error will vanish for  $L_2 \approx L$ . The main challenge will be a small overlap with adequate errors based on the amount of iterations.

## 4.2 Overlapping Schwarz wave form relaxation for a weakly coupled system of convection-diffusion-reaction equation

In the following part we are going to present the convergence and the error bound of the overlapping Schwarz wave form relaxation for the solution to the coupled system of convection-diffusion-reaction defined by two functions  $u_1$  and  $u_2$ . The coupling criteria in this case of study is imposed within the source term of the second solution component. The considered system with the solution  $u_1$  and  $u_2$  is given by

$$\begin{aligned} R_1 u_{1,t} &= D_1 u_{1,xx} - \nu_1 u_{1,x} - \lambda_1 u_1 \text{ over } \Omega = \{0 < x < L\}, \quad t \in [t_0, t_{\text{end}}], \\ u_1(0, t) &= f_{1,1}(t), \quad t \in [t_0, t_{\text{end}}], \\ u_1(L_2, t) &= f_{1,2}(t), \quad t \in [t_0, t_{\text{end}}], \\ u_1(x, t_0) &= u_0(x), \end{aligned} \tag{4.16}$$

for  $u_1$ , and for  $u_2$  is given by

$$\begin{aligned}
R_2 u_{2,t} &= D_2 u_{2,xx} - \nu_2 u_{2,x} - \lambda_2 u_2 + \lambda_1 u_1 \text{ over } \Omega, \quad t \in [t_0, t_{\text{end}}), \\
u_2(L_1, t) &= f_{2,1}(t), \quad t \in [t_0, t_{\text{end}}), \\
u_2(L, t) &= f_{2,2}(t), \quad t \in [t_0, t_{\text{end}}), \\
u_2(x, t_0) &= u_0(x).
\end{aligned} \tag{4.17}$$

For the uniqueness and existence of the equations (4.16) and (4.17) we apply theorem 4.1.

In (4.17) the coupling appears in the source term and is defined by the parameter  $\lambda_1$  with the first component  $u_1$ . The strength or the *bound* of the coupling and the contribution is related to the value of the scalar defined by  $\lambda_1$ . The coupled case (4.17) is reduced to the case of two decoupled equations by assuming  $\lambda_1 = 0$  in (4.17).

The overlapping Schwarz wave form relaxation for (4.16) over  $\Omega_1$  and  $\Omega_2$  is given by

$$\begin{aligned}
R_1 v_{1,t}^{k+1} &= D_1 v_{1,xx}^{k+1} - \nu_1 v_{1,x}^{k+1} - \lambda_1 v_1^{k+1} \text{ over } \Omega_1, \quad t \in [t_0, t_{\text{end}}), \\
v_1^{k+1}(0, t) &= f_{1,1}(t), \quad t \in [t_0, t_{\text{end}}), \\
v_1^{k+1}(L_2, t) &= \begin{cases} w_1^k(L_2, t) & \text{for } k > 1 \\ u_1(L_2, 0) & \text{for } k = 1 \end{cases}, \quad t \in [t_0, t_{\text{end}}), \\
v_1^{k+1}(x, t_0) &= u_0(x), \quad x \in \Omega_1,
\end{aligned} \tag{4.18}$$

$$\begin{aligned}
R_1 w_{1,t}^{k+1} &= D_1 w_{1,xx}^{k+1} - \nu_1 w_{1,x}^{k+1} - \lambda_1 w_1^{k+1} \text{ over } \Omega_2, \quad t \in [t_0, t_{\text{end}}), \\
w_1^{k+1}(L_1, t) &= \begin{cases} v_1^k(L_1, t) & \text{for } k > 1 \\ u_1(L_1, 0) & \text{for } k = 1 \end{cases}, \quad t \in [t_0, t_{\text{end}}), \\
w_1^{k+1}(L, t) &= f_{1,2}(t), \quad t \in [t_0, t_{\text{end}}), \\
w_1^{k+1}(x, t_0) &= u_0(x), \quad x \in \Omega_2.
\end{aligned} \tag{4.19}$$

For the system defined by (4.17) one denote the Schwarz wave form relaxation as

$$\begin{aligned}
R_2 v_{2,t}^{k+1} &= D_2 v_{2,xx}^{k+1} - \nu_2 v_{2,x}^{k+1} - \lambda_2 v_2^{k+1} + \lambda_1 v_1^{k+1} \text{ over } \Omega_1, \quad t \in [t_0, t_{\text{end}}), \\
v_2^{k+1}(0, t) &= f_{2,1}(t), \quad t \in [t_0, t_{\text{end}}), \\
v_2^{k+1}(L_2, t) &= \begin{cases} w_2^k(L_2, t) & \text{for } k > 1 \\ u_2(L_2, 0) & \text{for } k = 1 \end{cases}, \quad t \in [t_0, t_{\text{end}}), \\
v_2^{k+1}(x, t_0) &= u_0(x), \quad x \in \Omega_1,
\end{aligned} \tag{4.20}$$

$$\begin{aligned}
R_2 w_{2,t}^{k+1} &= D_2 w_{2,xx}^{k+1} - \nu_2 w_{2,x}^{k+1} - \lambda_2 w_2^{k+1} + \lambda_1 w_1^{k+1} \text{ over } \Omega_2, \quad t \in [t_0, t_{\text{end}}), \\
w_2^{k+1}(L_1, t) &= \begin{cases} v_2^k(L_1, t) & \text{for } k > 1 \\ u_2(L_1, 0) & \text{for } k = 1 \end{cases}, \quad t \in [t_0, t_{\text{end}}), \\
w_1^{k+1}(L, t) &= f_{2,2}(t), \quad t \in [t_0, t_{\text{end}}), \\
w_1^{k+1}(x, t_0) &= u_0(x), \quad x \in \Omega_2.
\end{aligned} \tag{4.21}$$

For the uniqueness and existence of the equations (4.18), (4.19), (4.20) and (4.21) we apply theorem 4.1.

The convergence and the error bound for the solution to (4.18-4.19) and (4.20- 4.21) is given by the following theorem.

**Theorem 4.3.** *Let  $e_i^{k+1}$  and  $d_i^{k+1}$  ( $i = 1, 2$ ) be the error from the solution to the subproblems (4.18-4.19) and (4.20- 4.21) by Schwarz wave form relaxation over  $\Omega_1$  and  $\Omega_2$ , respectively. Then the error bounds of (4.18)-(4.19) defined by  $e_1$  and  $d_1$  over  $\Omega_1$  and  $\Omega_2$  are given by*

$$\|e_1^{k+2}(L_1, \cdot)\|_\infty \leq \gamma_1 \|e_1^k(L_1, \cdot)\|_\infty, \quad (4.22)$$

and

$$\|d_1^{k+2}(L_1, \cdot)\|_\infty \leq \gamma_1 \|d_1^k(L_1, \cdot)\|_\infty, \quad (4.23)$$

respectively, and the error bound of (4.20- 4.21) defined by  $e_2$  and  $d_2$  over  $\Omega_1$  and  $\Omega_2$  are given by

$$\begin{aligned} \|e_2^{k+2}(L_1, \cdot)\|_\infty &\leq \|e_2^k(L_1, \cdot)\|_\infty \gamma_2 + \gamma_2 \frac{\lambda_1}{\lambda_2} \Psi \left[ 1 + e^{\alpha_2(L_1-L)} e^{\beta_2(L-L_1)} \right] \\ &+ \frac{\lambda_1}{\lambda_2} \Psi \left[ e^{\alpha_2(L_1-L_2)} \frac{\sinh \beta_2 L_1}{\sinh \beta_2 L_2} - e^{\alpha_2(L_1-L)} e^{\beta_2(L-L_2)} \frac{\sinh \beta_2 L_1}{\sinh \beta_2 L_2} \right] + \\ &\frac{\lambda_1}{\lambda_2} \Psi \left[ e^{\alpha_2 L_1} \frac{\sinh \beta_2 (L_1-L_2)}{\sinh \beta_2 L_2} - e^{\alpha_2(L_1-L_2)} \frac{\sinh \beta_2 L_1}{\sinh \beta_2 L_2} + 1 \right], \end{aligned} \quad (4.24)$$

and

$$\begin{aligned} \|d_2^{k+2}(L_2, \cdot)\|_\infty &\leq \|d_2^k(L_2, \cdot)\|_\infty \gamma_2 + \gamma_2 \frac{\lambda_1}{\lambda_2} \Psi \left[ 1 + e^{\alpha_2(L_1-L)} e^{\beta_2(L-L_1)} \right] \\ &+ \frac{\lambda_1}{\lambda_2} \Psi \left[ e^{\alpha_2(L_1-L_2)} \frac{\sinh \beta_2 L_1}{\sinh \beta_2 L_2} - e^{\alpha_2(L_1-L)} e^{\beta_2(L-L_2)} \frac{\sinh \beta_2 L_1}{\sinh \beta_2 L_2} \right] + \\ &\frac{\lambda_1}{\lambda_2} \Psi \left[ e^{\alpha_2 L_1} \frac{\sinh \beta_2 (L_1-L_2)}{\sinh \beta_2 L_2} - e^{\alpha_2(L_1-L_2)} \frac{\sinh \beta_2 L_1}{\sinh \beta_2 L_2} + 1 \right], \end{aligned} \quad (4.25)$$

respectively, where

$$\gamma_i = \frac{\sinh \beta_i L_1 \sinh \beta_i (L_2 - L)}{\sinh \beta_i L_2 \sinh \beta_i (L_1 - L)}, \quad \text{with} \quad \alpha_i = \frac{\nu_i}{2D_i}, \quad \beta_i = \frac{\sqrt{\nu_i^2 + 4D_i \lambda_i}}{2D_i},$$

for  $i = 1, 2$ , and  $\Psi = \max_\Omega \{e_1, e_2\}$ .

*Proof.* Since the system (4.16) does not depend on  $u_2$ , we can estimate the equations (4.22) and (4.23) by using the Theorem 4.2.

Let  $e_2^{k+1}(x, t) := u_2(x, t) - v_2^{k+1}(x, t)$  and  $d_2^{k+1}(x, t) := u_2(x, t) - w_2^{k+1}(x, t)$  be the error of (4.20) and (4.21) over  $\Omega_1$  and  $\Omega_2$  respectively. Then the corresponding

differential equations are satisfied by  $e_2(x, t)$  and  $d_2(x, t)$  :

$$\begin{aligned}
R_2 e_{2,t}^{k+1} &= D_2 e_{2,xx}^{k+1} - \nu_2 e_{2,x}^{k+1} - \lambda_2 e_2^{k+1} + \lambda_1 e_1^{k+1} \text{ over } \Omega_1, \quad t \in [t_0, t_{\text{end}}), \\
e_2^{k+1}(0, t) &= 0, \quad t \in [t_0, t_{\text{end}}), \\
e_2^{k+1}(L_2, t) &= d_2^k(L_2, t), \quad t \in [t_0, t_{\text{end}}), \\
e_2^{k+1}(x, t_0) &= 0, \quad x \in \Omega_2,
\end{aligned} \tag{4.26}$$

$$\begin{aligned}
R_2 d_{2,xx}^{k+1} &= D_2 d_{2,xx}^{k+1} - \nu_2 d_{2,x}^{k+1} - \lambda_2 d_2^{k+1} + \lambda_1 d_1^{k+1} \text{ over } \Omega_2, \quad t \in [t_0, t_{\text{end}}), \\
d_2^{k+1}(L_1, t) &= e_2^k(L_1, t), \quad t \in [t_0, t_{\text{end}}), \\
d_1^{k+1}(L, t) &= 0, \quad t \in [t_0, t_{\text{end}}), \\
d_1^{k+1}(x, t_0) &= 0, \quad x \in \Omega_2.
\end{aligned} \tag{4.27}$$

Furthermore we consider the following differential equations defined by  $\hat{e}^{k+1}$  and  $\hat{d}^{k+1}$  given by

$$\begin{aligned}
R_2 \hat{e}_{2,t}^{k+1} &= D_2 \hat{e}_{2,xx}^{k+1} - \nu_2 \hat{e}_{2,x}^{k+1} - \lambda_2 \hat{e}_2^{k+1} + \lambda_1 \Psi \text{ over } \Omega_1, \quad t \in [t_0, t_{\text{end}}), \\
\hat{e}_2^{k+1}(0, t) &= 0, \quad t \in [t_0, t_{\text{end}}), \\
\hat{e}_2^{k+1}(L_2, t) &= \|d_2^k(L_2, t)\|_{\Omega_2, \infty}, \quad t \in [t_0, t_{\text{end}}), \\
\hat{e}_2^{k+1}(x, t_0) &= \mathcal{A}(x), \quad x \in \Omega_1,
\end{aligned} \tag{4.28}$$

where  $\mathcal{A}(x)$  is given by

$$\begin{aligned}
\mathcal{A}(x) &= \|d_2^k(L_2, \cdot)\|_{\infty} e^{\alpha_2(x-L_2)} \frac{\sinh(\beta_2 x)}{\sinh(\beta_2 L)} \\
&\quad + \frac{\lambda_1}{\lambda_2} \Psi \left[ e^{\alpha_2 x} \frac{\sinh(\beta_2(x-L_2))}{\sinh(\beta_2 L_2)} - e^{\alpha_2(x-L_2)} \frac{\sinh \beta_2 x}{\sinh \beta_2 L_2} + 1 \right],
\end{aligned}$$

and

$$\begin{aligned}
R_2 \hat{d}_{2,t}^{k+1} &= D_2 \hat{d}_{2,xx}^{k+1} - \nu_2 \hat{d}_{2,x}^{k+1} - \lambda_2 \hat{d}_2^{k+1} + \lambda_1 \Psi \text{ over } \Omega_2, \quad t \in [t_0, t_{\text{end}}), \\
\hat{d}_2^{k+1}(L_1, t) &= \|e_2^k(L_1, t)\|_{\Omega_1, \infty}, \quad t \in [t_0, t_{\text{end}}), \\
\hat{d}_2^{k+1}(L, t) &= 0, \quad t \in [t_0, t_{\text{end}}), \\
\hat{d}_2^{k+1}(x, t_0) &= \mathcal{B}(x), \quad x \in \Omega_2,
\end{aligned} \tag{4.29}$$

where

$$\begin{aligned}
\mathcal{B}(x) &= \|e^k(L_1, \cdot)\|_{\infty} e^{\alpha_2(x-L_1)} \frac{\sinh(\beta_2(x-L))}{\sinh(\beta_2(L_1-L))} \\
&\quad + \frac{\lambda_1}{\lambda_2} \Psi \frac{\sinh(\beta_2(L-x))}{\sinh(\beta_2(L_1-L))} \left[ e^{\alpha_2(x-L_1)} - e^{\alpha_2(x-L)} e^{\beta_2(L-L_1)} \right] \\
&\quad - \frac{\lambda_1}{\lambda_2} \Psi \left[ 1 - e^{\alpha_2(x-L)} e^{\beta_2(L-x)} \right].
\end{aligned} \tag{4.30}$$

Then the solution to (4.28) and (4.29) is the steady state solution given by

$$\hat{e}_2^{k+1}(x, t) = \mathcal{A}(x), \quad \forall x \in \Omega_1, \quad t \in [t_0, t_{\text{end}}),$$

and

$$\hat{d}_2^{k+1}(x, t) = \mathcal{B}(x), \forall x \in \Omega_2, t \in [t_0, t_{\text{end}}],$$

respectively.

By defining the function  $E(x, t) = \hat{e}^{k+1} - e^{k+1}$ , as in the proof of theorem 4.2, and by the maximum principle theorem we conclude that

$$|e_2^{k+1}(x, t)| \leq \hat{e}_2^{k+1}(x, t)$$

for all  $(x, t)$  and similarly

$$|d_2^{k+1}(x, t)| \leq \hat{d}_2^{k+1}(x, t).$$

Then

$$\begin{aligned} \|e_2^{k+1}(x, \cdot)\|_\infty \leq & \|d_2^k(L_2, \cdot)\|_\infty e^{\alpha_2(x-L_2)} \frac{\sinh(\beta_2 x)}{\sinh(\beta_2 L)} \\ & + \frac{\lambda_1}{\lambda_2} \Psi \left[ e^{\alpha_2 x} \frac{\sinh(\beta_2(x-L_2))}{\sinh(\beta_2 L_2)} - e^{\alpha_2(x-L_2)} \frac{\sinh \beta_2 x}{\sinh \beta_2 L_2} + 1 \right], \end{aligned} \quad (4.31)$$

and

$$\begin{aligned} \|d_2^{k+1}(x, t)\|_\infty \leq & \|e^k(L_1, \cdot)\|_\infty e^{\alpha_2(x-L_1)} \frac{\sinh(\beta_2(x-L))}{\sinh(\beta_2(L_1-L))} \\ & + \frac{\lambda_1}{\lambda_2} \Psi \frac{\sinh(\beta_2(L-x))}{\sinh(\beta_2(L_1-L))} \left[ e^{\alpha_2(x-L_1)} - e^{\alpha_2(x-L)} e^{\beta_2(L-L_1)} \right] - \\ & \frac{\lambda_1}{\lambda_2} \Psi \left[ 1 - e^{\alpha_2(x-L)} e^{\beta_2(L-x)} \right]. \end{aligned} \quad (4.32)$$

By evaluating (4.32) for  $d_2^k(x, t)$  at  $x = L_2$ , substituting the results in (4.31) and afterwards evaluating the resulting relation at  $x = L_1$  we observe that (4.24) holds in general.

Similarly (4.25) follows from evaluating  $e_2^{k+1}(x, t)$  at  $x = L_1$ , substituting in (4.32) and evaluating afterwards the resulting relation at  $x = L_2$ .  $\square$

For the coupled system we observed the Theorem 4.3 and assume that the error depends on two main factors, the convergence parameter  $\gamma_i$  and the coupling parameter  $\lambda_1$  defining the system coupling (4.16), (4.17). Its obvious that for the coupling parameter  $\lambda_1 = 0$  one retain the decoupled system and faster convergence rate is achieved if we have a small ratio  $\frac{\lambda_1}{\lambda_2}$ .

## 5 Numerical Results

In this section we will present the numerical results from the solution to several model problems using the presented methods. The problems are discretized using

second order approximation with respect to the spatial variable using regular mesh spacing  $h(= L/N)$  and backward approximation with respect to the time using  $\Delta t$  time stepping. The first order operator splitting method (FOP) is considered to be the basic solution algorithm for the overlapping Schwarz waveform relaxation method (FOPSWR).

## 5.1 First example : Convection-diffusion-reaction equation

We consider the one-dimensional convection-diffusion-reaction equation given by

$$R\partial_t u + v\partial_x u - \partial_x D\partial_x u = -\lambda u, \text{ on } \Omega \times [t_0, t_{\text{end}}] \quad (5.1)$$

$$u(x, t_0) = u_{\text{exact}}(x, t_0), \quad (5.2)$$

$$u(0, t) = u_{\text{exact}}(0, t), \quad u(L, t) = u_{\text{exact}}(L, t), \quad (5.3)$$

defined over  $\Omega \times [t_0, t_{\text{end}}]$  with  $\Omega = [0, L]$ , and  $t_0 = 100$ ,  $t_{\text{end}} = 10^5$  and  $L = 150$ . Further we have  $\lambda = 10^{-5}$ ,  $v = 0.001$ ,  $D = 0.0001$  and  $R = 1.0$ .

The analytical solution of the equation (5.1) considered on  $\mathbb{R} \times (0, t_{\text{end}})$ , with vanishing Dirichlet-boundary conditions and also using a  $\delta$ -function as initial value, can be derived by Laplace-Transformation, see [15], and is given by

$$u_{\text{exact}}(x, t) = \frac{\tilde{u}_0}{2\sqrt{D\pi t}} \exp\left(-\frac{(x - vt)^2}{4Dt}\right) \exp(-\lambda t), \quad (5.4)$$

with  $\tilde{u}_0 = 1$ , the restriction of  $u_{\text{exact}}$  to  $\Omega \times (0, t_{\text{end}})$  is a solution to (5.1)-(5.3).

We considered the backward Euler discretization for both of the splitted operators, i.e. the convection and the diffusion reaction operator, to simulate the solution over the time interval  $[100, 10^5]$ .

The model problem (5.1) is solved using first order operator splitting (FOP), and also the operator splitting with overlapping Schwarz wave form relaxation method (FOPSWR).

We compare the accuracy of the solution over the entire spatial domain with different  $h$  values, and different time steps  $\Delta t$ , using FOP-method, and FOPSWR-method over two subdomains with different size of overlapping. The error of solution are given in Table 1, and Table 2, respectively. The FOPSWR-method is considered over two overlapping subdomains of different overlapping size  $L_2 - L_1$ , to conclude on the accuracy of the algorithm with the operator splitting. The considered subdomains were  $\Omega_1 = [0, 60]$ , and  $\Omega_2 = [30, 150]$  and  $\Omega_1 = [0, 100]$ , and  $\Omega_2 = [30, 150]$

The results derived for the FOP-method are presented the in Figure 1.

In the numerical computations the time-steps and space-steps are systematically refined in order to visualize the accuracy and error reduction through the simulation over the time interval for refined time and space steps. From Table 1 one observes that by the FOP-method the error reduced as second order with respect to space



time	err <sub>u<sub>1</sub></sub>	err <sub>u<sub>1</sub></sub>	err <sub>u<sub>1</sub></sub>
$\Delta t_0 = 20$	0.001195	2.86514e-4	1.2868e-4
$\Delta t_0/2 = 10$	0.00113	2.3942e-4	8.6641e-5
$\Delta t_0/4 = 5$	0.001108	2.15813e-4	6.55262e-5
	$h_0 = 1$	$h = h_0/2$	$h = h_0/4$

Table 1: The  $L_{\Omega,\infty}$ -error in time and space for the convection-diffusion-reaction-equation using FOP-method.

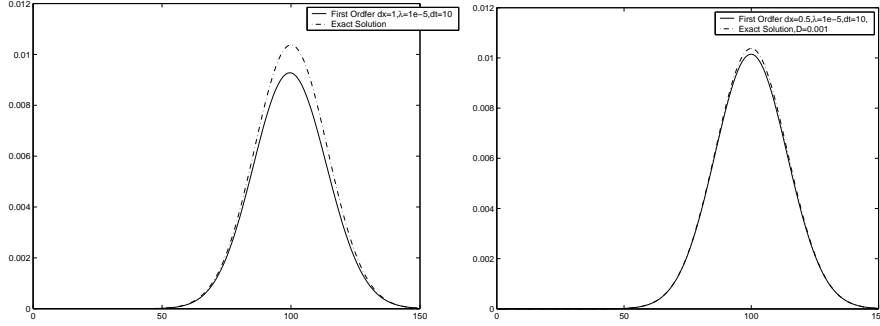


Figure 1: The results for the FOP-method.

time	err <sub>u<sub>1</sub></sub>	err <sub>u<sub>1</sub></sub>	err <sub>u<sub>1</sub></sub>	err <sub>u<sub>1</sub></sub>	err <sub>u<sub>1</sub></sub>	err <sub>u<sub>1</sub></sub>
$\Delta t_0 = 20$	1.196e-3	1.195e-3	2.871e-4	2.865e-4	1.290e-4	1.286e-4
$\Delta \frac{t_0}{2} = 10$	1.138e-3	1.137e-3	2.397e-4	2.394e-4	8.681e-5	8.681e-5
$\Delta \frac{t_0}{4} = 5$	1.108e-3	1.08e-3	2.159e-4	2.158e-4	6.782e-5	6.552e-5
overlap.	30	70	30	70	30	70
size	$h_0 = 1$		$h = h_0/2$		$h = h_0/4$	

Table 2: The  $L_{\Omega,\infty}$ -error in time and space for the scalar convection-diffusion-reaction-equation using FOPSWR- method with the Schwarz waveform relaxation algorithm for two different size of overlapping 30 and 70.

and reduced also with respect to time. For further refinement one should obtain first order convergence results with respect to time.

For the solution by the FOPSWR-method, using the FOP-method as basic solver, the accuracy of the solution is improved over the large size of overlapping subdomains.

The results for the modified method are presented in the Figure 2.

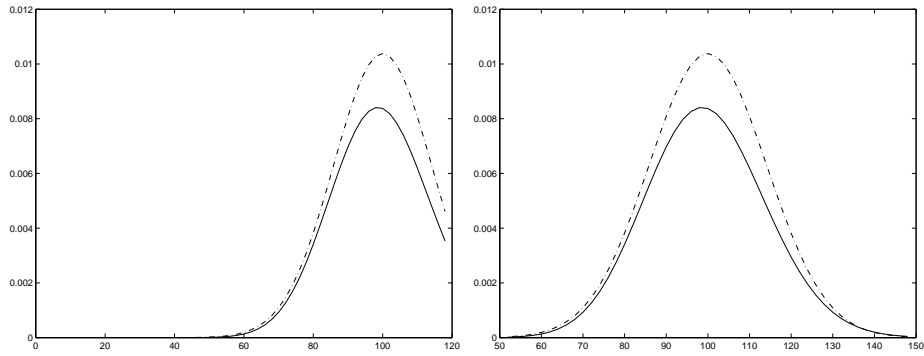


Figure 2: The results for the Schwarz-method with 2 domains (overlapping 30).

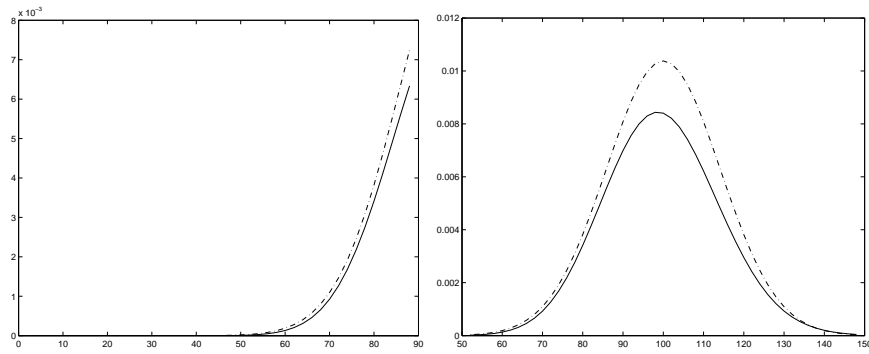


Figure 3: The results for the Schwarz-method with 2 domains (overlapping 70).

## 5.2 Second example System of Convection-diffusion-reaction equation

We consider a further example of a one-dimensional convection-diffusion-reaction equation, given as (5.1) - (5.4) with the following parameters  $\lambda = 4.0 \cdot 10^{-5}$ ,  $v = 0.001$ ,  $D = 0.0001$ ,  $R = 1.0$  and  $t_0 = 100$ .

For the initial condition we use the analytical solution given in (5.4), with  $\tilde{u}_0 = 1.0$  and  $t_0 = 100$ . As boundary condition we use the Dirichlet-Boundary-condition with the analytical solutions given in (5.4). The time-interval is  $[100, 10^5]$ .

The results for the classical method (operator-splitting) are given in Table 3.

time	err <sub>u<sub>1</sub></sub>	err <sub>u<sub>1</sub></sub>	err <sub>u<sub>1</sub></sub>
$\Delta t = 20$	2.075e-4	1.963e-4	1.799e-4
$\Delta \frac{t}{2} = 10$	2.055e-4	1.948e-4	1.794e-4
$\Delta \frac{t}{4} = 5$	2.045e-4	1.940e-4	1.792e-4
size	$h_0 = 1$	$h = h_0/2$	$h = h_0/4$

Table 3:  $L_{\Omega, \infty}$ -error in time and space for the convection-diffusion-reaction equation solved by operator splitting.

In the next experiments we consider the modified method. For the overlapping we obtain the overlap size-length of 30 and 70, i.e.  $\Omega_1 = \{0 < x < 60\}$  and  $\Omega_2 = \{30 < x < 150\}$  while for the other case we have  $\Omega_1 = \{0 < x < 100\}$  and  $\Omega_2 = \{30 < x < 150\}$ .

The results are given in Table 4.

time	err <sub>u<sub>1</sub></sub>	err <sub>u<sub>1</sub></sub>	err <sub>u<sub>1</sub></sub>	err <sub>u<sub>1</sub></sub>	err <sub>u<sub>1</sub></sub>	err <sub>u<sub>1</sub></sub>
$\Delta t_0 = 20$	2.076e-4	2.075e-3	1.964e-4	1.963e-4	1.800e-4	1.800e-4
$\Delta \frac{t_0}{2} = 10$	2.056e-4	2.055e-4	1.948e-4	1.948e-4	1.795e-4	1.794e-4
$\Delta \frac{t_0}{4} = 5$	2.046e-4	2.046e-3	1.941e-4	1.941e-4	1.792e-4	1.792e-5
overlap.	30	70	30	70	30	70
size	$h_0 = 1$		$h = h_0/2$		$h = h_0/4$	

Table 4: The  $L_{\Omega, \infty}$ -error in time and space for the scalar convection-diffusion-reaction-equation using DD for two different size of overlapping 30 and 70 and operator splitting.

We compare the results of our computations given in Table (3) and (4). We can observe a reduction of the error for each time and space refinement for the modified method. Further refinement in time would obtain a first order convergence result. Because of the decoupling, each equation could be computed separately. For the first component one derive improved results because of the smaller reaction in the equation.

### 5.3 Third example System of Convection-diffusion-reaction equation (coupled), solved with Operator-Splitting

We deal with the more complicate example of a one-dimensional convection-diffusion-reaction equation.

$$R_1 \partial_t u_1 + v \partial_x u_1 - \partial_x D \partial_x u_1 = -R_1 \lambda_1 u_1, \quad (5.5)$$

$$R_2 \partial_t u_2 + v \partial_x u_2 - \partial_x D \partial_x u_2 = R_1 \lambda_1 u_1 - R_2 \lambda_2 u_2, \quad (5.6)$$

$$u_1(x, t_0) = u_{1,\text{exact}}(x, t_0), u_2(x, t_0) = u_{2,\text{exact}}(x, t_0) \quad (5.7)$$

$$u_1(0, t) = u_{1,\text{exact}}(0, t), u_2(0, t) = u_{2,\text{exact}}(0, t), \quad (5.8)$$

$$u_1(L, t) = u_{1,\text{exact}}(L, t), u_2(L, t) = u_{2,\text{exact}}(L, t), \quad (5.9)$$

defined over  $\Omega \times [t_0, t_{\text{end}}]$  with  $\Omega = [0, L]$ , and  $t_0 = 100$ ,  $t_{\text{end}} = 10^5$  and  $L = 150$ . Further we have  $\lambda_1 = 1.0 \cdot 10^{-5}$ ,  $\lambda_2 = 4.0 \cdot 10^{-5}$ ,  $v = 0.001$ ,  $D = 0.0001$ ,  $R_1 = 2.0$ , and  $R_2 = 1.0$ .

The analytical solution of the equation (5.5)-(5.6) considered on  $\mathbb{R} \times (0, t_{\text{end}})$ , with vanishing Dirichlet-boundary conditions and also using a  $\delta$ -function as initial value, can be derived by Laplace-Transformation, see [15], and is given by

$$u_{1,\text{exact}}(x, t) = \frac{u_{10}}{2R_1 \sqrt{D \pi t/R_1}} e^{-\frac{(x-vt/R_1)^2}{4D t/R_1}} e^{-\lambda_1 t},$$

$$\begin{aligned} u_{2,\text{exact}}(x, t) &= \frac{u_{20}}{2R_2 \sqrt{D \pi t/R_2}} e^{-\frac{(x-vt/R_2)^2}{4D t/R_2}} e^{-\lambda_2 t} \\ &+ \frac{R_1 \lambda_1 u_{10}}{2\sqrt{D \pi (R_1 - R_2)}} \exp\left(\frac{xv}{2D}\right) e^{-\frac{(R_1 \lambda_1 - R_2 \lambda_2) t}{(R_1 - R_2)}} (W(\nu_2) - W(\nu_1)), \end{aligned}$$

$$\nu_1 = \sqrt{R_1 \lambda_1 - \frac{(R_1 \lambda_1 - R_2 \lambda_2)}{R_1 - R_2} R_1 + v^2/(4D)},$$

$$\nu_2 = \sqrt{R_2 \lambda_2 - \frac{(R_1 \lambda_1 - R_2 \lambda_2)}{R_1 - R_2} R_2 + v^2/(4D)},$$

$$W(\nu) = 0.5(\exp(-\frac{xv\nu}{2D})\text{erfc}(\frac{x-v\nu t}{\sqrt{4Dt}}) + \exp(\frac{xv\nu}{2D})\text{erfc}(\frac{x+v\nu t}{\sqrt{4Dt}})),$$

defined for the initial condition with  $u_{10} = 1.0$  and  $u_{20} = 0.0$ , the restriction of  $u_{\text{exact}}$  to  $\Omega \times (0, t_{\text{end}})$ .

We have  $\text{erfc}(\cdot)$  as the known error-function and we denote the following conditions :  $R_1 > R_2$  and  $\lambda_2 > \lambda_1$ .

In the next tables we compare the classical with the modified method and test the depend on the reaction-parameters.

time	err <sub>u<sub>1</sub></sub>	err <sub>u<sub>2</sub></sub>	err <sub>u<sub>1</sub></sub>	err <sub>u<sub>2</sub></sub>	err <sub>u<sub>1</sub></sub>	err <sub>u<sub>2</sub></sub>
$\Delta t_0 = 20$	4.594e-4	2.8e-3	3.611e-4	2.452e-3	1.036e-4	2.702e-3
$\Delta \frac{t_0}{2} = 10$	4.506e-4	2.403e-3	3.515e-4	2.447e-3	9.528e-5	2.697e-3
$\Delta \frac{t_0}{4} = 5$	4.461e-4	2.39e-3	3.466e-4	2.438e-3	9.110e-5	2.689e-3
size	$h_0 = 1$		$h = h_0/2$		$h = h_0/4$	

Table 5:  $L_{\Omega, \infty}$ -error in time and space for the system of convection-diffusion-reaction-equation using first order splitting, with  $\lambda_1 = 2e - 5$ ,  $\lambda_2 = 4e - 5$ .

The results for the classical method (Operator-Splitting method) are given in Table 5.

The results for the modified method (Operator-Splitting method and Domain decomposition method) is given in Table 6.

time	err <sub>u<sub>1</sub></sub>	err <sub>u<sub>2</sub></sub>	err <sub>u<sub>1</sub></sub>	err <sub>u<sub>2</sub></sub>	err <sub>u<sub>1</sub></sub>	err <sub>u<sub>2</sub></sub>
$\Delta t_0 = 20$	4.594e-4	2.403e-3	3.611e-4	2.452e-3	1.036e-4	2.702e-3
$\Delta \frac{t_0}{2} = 10$	4.506e-4	2.398e-3	3.515e-4	2.447e-3	9.528e-5	2.697e-3
$\Delta \frac{t_0}{4} = 5$	4.461e-4	2.388e-3	3.466e-4	2.438e-3	9.110e-5	2.689e-3
size	$h_0 = 1$		$h = h_0/2$		$h = h_0/4$	
overlap.	70					

Table 6:  $L_{\Omega, \infty}$ -error in time and space for the system of convection-diffusion-reaction-equation using first order splitting and Schwarz wave form relaxation method, with  $\lambda_1 = 2e - 5$ ,  $\lambda_2 = 4e - 5$ .

In the Figure 4 one sees the result for the system, where the solutions for different time-steps are presented.

We modify for a second experiment the reaction-parameters to obtain the influence between the first and the second component. In the first computation we use the classical method and get the following results given in Table 7.

time	err <sub>u<sub>1</sub></sub>	err <sub>u<sub>2</sub></sub>	err <sub>u<sub>1</sub></sub>	err <sub>u<sub>2</sub></sub>	err <sub>u<sub>1</sub></sub>	err <sub>u<sub>2</sub></sub>
$\Delta t = 20$	3.396e-3	6.058e-7	2.673e-3	6.192e-7	7.746e-4	6.820e-7
$\Delta \frac{t}{2} = 10$	3.30e-3	6.044e-7	2.599e-3	6.179e-7	7.083e-4	6.808e-7
$\Delta \frac{t}{4} = 5$	3.297e-3	6.018e-7	2.562e-3	6.152e-7	6.753e-4	6.784e-7
size	$h_0 = 2$		$h = h_0/2$		$h = h_0/4$	

Table 7:  $L_{\Omega, \infty}$ -error in time and space for the system of convection-diffusion-reaction-equation using first order splitting, with  $\lambda_1 = 1e - 9$ ,  $\lambda_2 = 4e - 5$ .

In the second computation we use the modified method and get the following results

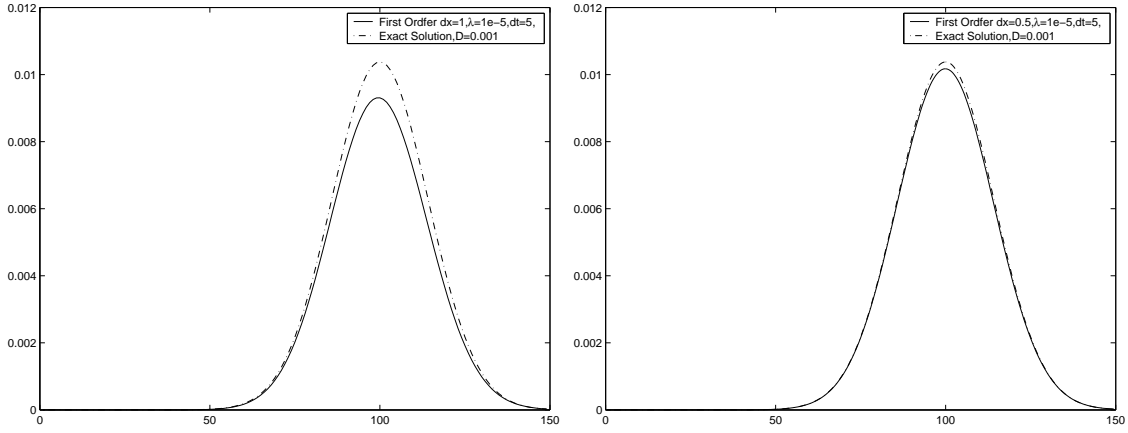


Figure 4: The first-order results for the different time-steps and discretisations for the first component and different time-steps.

given in Table 8.

time	err <sub>u<sub>1</sub></sub>	err <sub>u<sub>2</sub></sub>	err <sub>u<sub>1</sub></sub>	err <sub>u<sub>2</sub></sub>	err <sub>u<sub>1</sub></sub>	err <sub>u<sub>2</sub></sub>
$\Delta t = 20$	3.380e-3	6.058e-7	2.673e-3	6.192e-7	7.746e-4	6.820e-7
$\Delta \frac{t}{2} = 10$	3.314e-3	6.044e-7	2.599e-3	6.179e-7	7.083e-4	6.808e-7
$\Delta \frac{t}{4} = 5$	3.297e-3	6.018e-7	2.545e-3	6.152e-7	6.753e-4	6.784e-7
size	$h_0 = 2$		$h = h_0/2$		$h = h_0/4$	
overlap.	70					

Table 8:  $L_{\Omega, \infty}$ -error in time and space for the system of convection-diffusion-reaction-equation using first order splitting and Schwarz wave form relaxation method with  $\lambda_1 = 1e - 9$ ,  $\lambda_2 = 4e - 5$ .

We see in Table 7 and 8 a higher order results in space for the first component. For the second component the influence of the first component is important and decreasing the error of the first component, also decreases the error of the second component. The results for the modified method are shown in the Figure 5.

In the next section we present our conclusions.

## 6 Conclusions and Discussions

We present the mathematical background for the coupling of simple physical and one-dimensional software-codes. The convergence-results for simple and systems of one-dimensional parabolic equations are derived for the Schwarz-Domain-Decomposition-method. Numerical results for the scalar and system of parabolic equations are done and we can see the effectivity with Domain-Decomposition and Operator-Splitting-

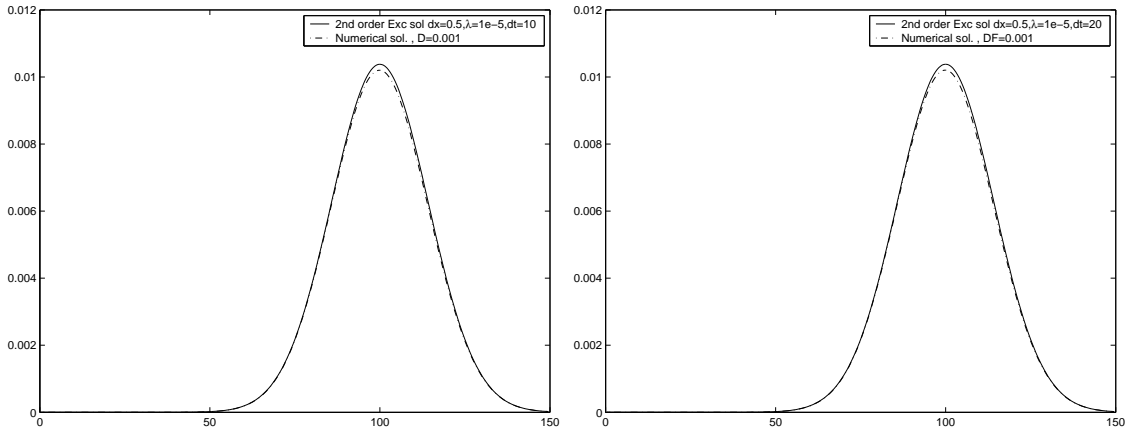


Figure 5: The second-order results for the different time-steps and discretisations for the first component and different time-steps.

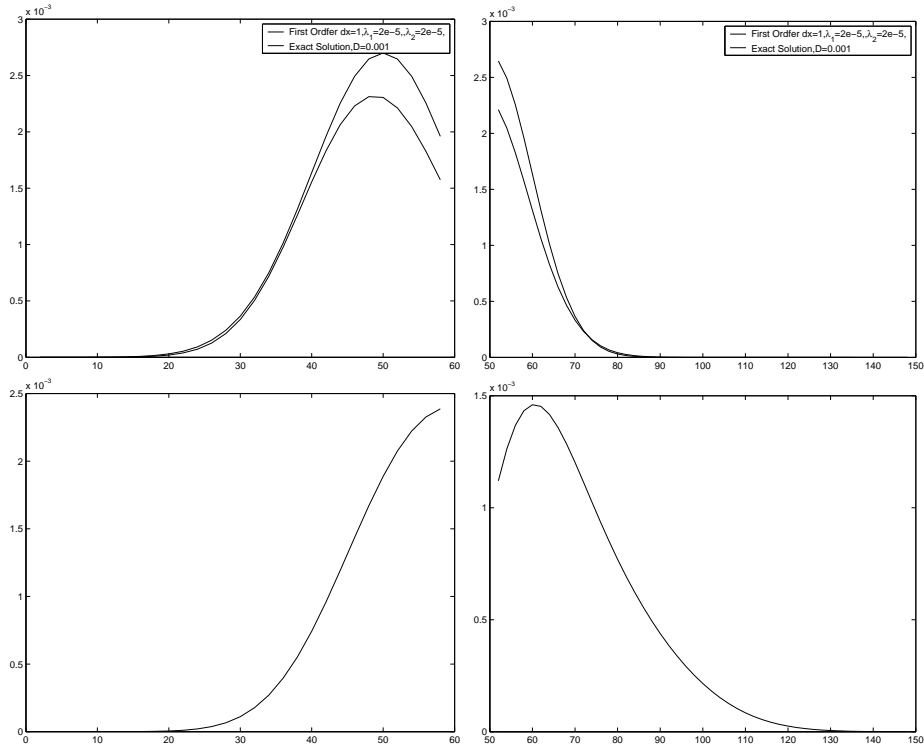


Figure 6: The results for the Schwarz-method with 2 domains.

methods. In future we will focus on more applied problems, for example in crystal-growth, see [1] and biological models, see [6].

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