Manuscript submitted to
AIMS' Journals
Volume **X**, Number **0X**, XX **200X**

Website: http://AIMsciences.org

pp. **X–XX**

SCHWARZ WAVEFORM RELAXATION ALGORITHMS FOR SEMILINEAR REACTION-DIFFUSION EQUATIONS

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(Communicated by the associate editor name)

Abstract. We introduce nonoverlapping domain decomposition algorithms of Schwarz waveform relaxation type for the semilinear reaction-diffusion equation. We define linear Robin and second order (or Ventcell) transmission conditions between the subdomains, which we prove to lead to a well defined and converging algorithm. We also propose nonlinear transmission conditions. Both types are based on best approximation problems for the linear equation and provide efficient algorithms, as the numerical results that we present here show.

1. **Introduction.** For reactive transport modeling in a CO_2 geological storage modeling context, one is especially interested in the long-term behavior of the injected chemical substances with regard to large spatial dimensions. Our angle of vision is several hundreds, even thousands of years in time and several hundreds, even thousands of meters in space. Simulating geological storage processes is subject to the following challenges: for performance reasons, general calculations have to be done with large temporal and spatial dimensions because the chemical system is expected to become quickly equalized on account of slow flow rate in comparison to fast reaction rates. However, in front areas, where concentration gradients are significantly elevated, the chemical system is highly unequalized and has then to be solved with high accuracy in time and space. Therefore, the approach is a coarse time mesh integration scheme with refined areas in time and space around the reaction fronts. For later works, one challenge is to detect and track those reaction

2000 *Mathematics Subject Classification.* 35K55, 65M12, 65M55.

Key words and phrases. Domain decomposition, Schwarz waveform relaxation, Semilinear reaction-diffusion equation, Nonlinear transmission conditions.

This research is supported by the research project SHPCO2 funded by ANR-07-CIS7-007-03.

areas as well as the local time-step and grid size adaptation coupled with a domain decomposition method in order to solve the problem with higher performance by avoiding bad convergence of the linear solvers and small time steps for non-reactive areas. Those works are in the general claim for parallelism, in order to be able to treat numerically realistic cases with more than 100.000 cells in reasonable time (less than one day)[9].

The SHPCO$_2$ project (High Performance Simulation of CO$_2$ Geological Storage [12]) considers as a main tool for space-time refinement the Schwarz waveform relaxation algorithms. These algorithms were proposed in a linear setting in [2], [4], [6], [11]. They solve space-time problems alternatively in the subdomains. The exchange of information between the subdomains is done by boundary transmission operators, like Robin operators or Ventcell operators. Therefore they are very-well suited for different space and time discretizations in the subdomains [10]. The transmission conditions are optimized through certain coefficients, which in certain cases can be obtained in asymptotic closed form ([2], [6]).

However, in the project the equations are nonlinear, and new algorithms must be designed in this context. Overlapping Schwarz waveform relaxation algorithms, exchanging information through Dirichlet data, were proposed in [8] for the Burgers equation. The purpose of the present paper is to set a theory for more efficient algorithms for the semilinear heat equation, using the above described transmission conditions.

The paper is structured as follows: we first present the problem and the nonoverlapping Schwarz waveform relaxation algorithm in Section 2. We also state the theoretical results: definition of the algorithm, existence of a common existence time for the nonlinear problems, convergence of the algorithm.

Section 3 is devoted to the proof of these results.

Section 4 presents the numerical treatment of the subdomain problems, and of the algorithm.

Finally Section 5 quantifies the theoretical convergence result.

2. **Problem description.**

We consider a semilinear reaction diffusion equation in two dimensions,

$$u_t - \nu\Delta u + f(u) = 0, \text{ in } \mathbb{R}^2 \times (0, T), \tag{1}$$

with initial condition

$$u(\cdot, 0) = u_0, \tag{2}$$

where $T > 0$ and the diffusion coefficient ν is a strictly positive constant. The function f defining the nonlinearity is in $\mathcal{C}^2(\mathbb{R})$, and satisfies $f(0) = 0$. The initial data u_0 is supposed to be defined in $H^2(\mathbb{R}^2)$.

A weak solution of problem (1)-(2) is defined to be a function $u \in L^2(0, T; H^1(\mathbb{R}^2)) \cap \mathcal{C}([0, T]; L^2(\mathbb{R}^2))$, such that $f(u) \in L^2(0, T; L^2(\mathbb{R}^2))$, satisfying for all $v \in H^1(\mathbb{R}^2)$

$$\frac{d}{dt}(u, v) + \nu(\nabla u, \nabla v) + (f(u), v) = 0, \quad \text{in } \mathcal{D}'(0, T),$$

and $u(\cdot, 0) = u_0$, where $(\cdot, \cdot)$ denotes the inner product in $L^2(\mathbb{R}^2)$.

Let us recall the following result concerning the well-posedness of the Cauchy problem (1)-(2) (for a proof, see for instance [3]):

Theorem 2.1. *If $u_0 \in H^2(\mathbb{R}^2)$, then there exists $T > 0$ such that problem (1)-(2) possesses a unique weak solution $u \in L^2(0, T; H^1(\mathbb{R}^2)) \cap \mathcal{C}([0, T]; L^2(\mathbb{R}^2))$. We have in addition that $u \in L^\infty(0, T; H^2(\mathbb{R}^2))$.*

We introduce a nonoverlapping Schwarz waveform relaxation algorithm to approximate the solution u of problem (1)-(2). We decompose the domain $\mathbb{R}^2$ into two subdomains $\Omega_1 = (-\infty, 0) \times \mathbb{R}$ and $\Omega_2 = (0, +\infty) \times \mathbb{R}$. We denote by $\Gamma := \{0\} \times \mathbb{R}$ the common boundary of Ω_1 and Ω_2 and by $n_1 = (1, 0)$ and $n_2 = (-1, 0)$ respectively the unit outward normal vectors to Ω_1 and Ω_2 at Γ. The nonoverlapping Schwarz waveform relaxation algorithm is given by:

$$\begin{cases} \partial_t u_1^k - \nu \Delta u_1^k + f(u_1^k) = 0, & \text{in } \Omega_1 \times (0, T), \\ u_1^k(\cdot, 0) = u_{0|\Omega_1}, & \text{in } \Omega_1, \\ B_1(u_1^k) = B_1(u_2^{k-1}), & \text{over } \Gamma \times (0, T), \end{cases} \tag{3}$$

and

$$\begin{cases} \partial_t u_2^k - \nu \Delta u_2^k + f(u_2^k) = 0, & \text{in } \Omega_2 \times (0, T), \\ u_2^k(\cdot, t = 0) = u_{0|\Omega_2}, & \text{in } \Omega_2, \\ B_2(u_2^k) = B_2(u_1^{k-1}), & \text{over } \Gamma \times (0, T), \end{cases} \tag{4}$$

where B_1 and B_2 are differential operators to be defined.

An initial guess (g_1^0, g_2^0) is given. At step 0 of the algorithm we solve both problems (3) and (4) with transmission conditions replaced respectively by the conditions

$$B_1(u_1^0) = g_1^0 \quad \text{and} \quad B_2(u_2^0) = g_2^0. \tag{5}$$

The transmission operators are either

$$B_i(u) = \nu \frac{\partial u}{\partial n_i} + pu \tag{6}$$

for positive p, or

$$B_i(u) = \nu \frac{\partial u}{\partial n_i} + pu + q\Big(\frac{\partial u}{\partial t} - \nu \frac{\partial^2 u}{\partial y^2}\Big) \tag{7}$$

for positive p and q. We refer to operators (6) as Robin operators, and operators (7) as Ventcell operators. They have been designed and studied in a linear setting in [2], [6], as approximations of the Dirichlet-Neumann operators, thus leading to optimized convergence of the algorithm for cleverly chosen coefficients p and q. They were obtained by a Fourier transform in time and in the direction y of the interface.

We define the algorithm in the frame of Sobolev spaces. We denote by $(\cdot, \cdot)$ the inner product in $L^2(\Omega_i)$ and by $(\cdot, \cdot)_\Gamma$ the inner product in $L^2(\Gamma)$. For $s \geq 1$, we introduce the function spaces

$$H_s^s(\Omega_i) = \{u \in H^s(\Omega_i),\ u_{|\Gamma} \in H^s(\Gamma)\},$$

$V = H^1(\Omega_i)$, if $q = 0$, and $V = H_1^1(\Omega_i)$, if $q > 0$. If $g \in L^2(0, T; H^{\frac{1}{2}}(\Gamma))$ is given, a weak solution of the boundary value problem

$$\begin{cases} w_t - \nu \Delta w + f(w) = 0, & \text{in } \Omega_i \times (0, T), \\ w(\cdot, 0) = u_{0|\Omega_i}, & \text{in } \Omega_i, \\ \nu \dfrac{\partial w}{\partial n_i} + pw + q(\dfrac{\partial w}{\partial t} - \nu \dfrac{\partial^2 w}{\partial y^2}) = g, & \text{over } \Gamma \times (0, T), \end{cases} \tag{8}$$

is a function $w \in L^2(0, T; V)$ such that for all $v \in V$,

$$\frac{d}{dt}(w, v) + \nu(\nabla w, \nabla v) + p(w, v)_\Gamma + q\frac{d}{dt}(w, v)_\Gamma + \nu q(\frac{\partial w}{\partial y}, \frac{\partial v}{\partial y})_\Gamma + (f(w), v) = (g, v)_\Gamma, \tag{9}$$

in $\mathcal{D}'(0,T)$, and such that $w_{|t=0} = u_{0|\Omega_i}$.

The first result is a local well-posedness result for the algorithm:

Theorem 2.2. *Let g_1^0 and g_2^0 in $H^1(0,T;L^2(\Gamma)) \cap L^\infty(0,T;H^{\frac{1}{2}}(\Gamma))$, $u_0 \in H^2(\mathbb{R}^2)$, $p>0$ and $q \geq 0$ be given. Suppose that $(\nu\partial_{n_i}u_0 + pu_0)|_\Gamma = g_i^0(0,\cdot)$, if $q=0$. Then, algorithm (3)-(4) with the transmission operators defined by (7) (or by (6) if $q=0$), initialized with (5), defines a unique sequence of iterates (u_1^k, u_2^k) such that*

$$u_i^k \in W^{1,\infty}(0,T_k;L_2(\Omega_i)) \cap L^\infty(0,T_k;H_2^2(\Omega_i)) \cap H^1(0,T_k;H^1(\Omega_i)),$$

if $q>0$, or such that

$$u_i^k \in W^{1,\infty}(0,T_k;L_2(\Omega_i)) \cap L^\infty(0,T_k;H^2(\Omega_i)) \cap H^1(0,T_k;H^1(\Omega_i)),$$

if $q=0$, for some T_k, $0<T_k\leq T$.

The second result shows that the iterates have indeed an existence time independent of k.

Theorem 2.3. *Under the conditions of Theorem 2.2, there exists $\overline{M}$ and $\overline{T}$ such that, if*

$$\|u_0\|^2_{H^2(\Omega_i)} + \|g_i^0\|^2_{H^1(0,\overline{T};L^2(\Gamma))\cap L^\infty(0,\overline{T};H^{\frac{1}{2}}(\Gamma))} \leq \overline{M}^{\,2}, \tag{10}$$

(u_1^k, u_2^k) is defined in the interval $[0,\overline{T}\,]$ for all positive k.

The third result shows the convergence of the algorithm.

Theorem 2.4. *With the notations of Theorem 2.3, the sequence (u_1^k, u_2^k) converges, as $k\to\infty$, to $(u_{|\Omega_1}, u_{|\Omega_2})$, in $L^\infty(0,\overline{T};H^1(\Omega_i))$.*

3. **Proofs of the theorems.** All proofs are given in the case $q=0$. The proofs in the Ventcell case are much more technical, but follow the same path.

3.1. **Proof of theorem 2.2.** In a first step we prove existence and uniqueness of the solution for the non-homogeneous linear problem associated with (8) in some regular space in which $f(w)$ is well-defined. This proof is inspired by [13], where absorbing boundary conditions are considered, *i*.e. with $g=0$.

We then define the solution of the nonlinear problem by using the Picard fixed point theorem in some suitable metric space.

We introduce the linear problem

$$\begin{cases} w_t - \nu\Delta w = \tilde{f}, & \text{in } \Omega_i \times (0,T),\\ w(\cdot,\cdot,0) = u_{0|\Omega_i}, & \text{in } \Omega_i,\\ \nu\frac{\partial w}{\partial n_i} + pw = g, & \text{over } \Gamma\times(0,T). \end{cases} \tag{11}$$

Lemma 3.1. *Let u_0 in $H^2(\Omega_i)$, $\tilde{f} \in H^1(0,T;L^2(\Omega))$ and $g \in H^1(0,T;L^2(\Gamma)) \cap L^\infty(0,T;H^{\frac{1}{2}}(\Gamma))$ such that $\nu\frac{\partial u_0}{\partial n_i}(\cdot) + pu_0(\cdot) = g(0,\cdot)$ over Γ. Then problem (11) has a unique solution in*

$$\mathcal{H}(T) := W^{1,\infty}(0,T;L^2(\Omega_i)) \cap L^\infty(0,T;H^2(\Omega_i)) \cap H^1(0,T;H^1(\Omega_i)). \tag{12}$$

and the following estimate holds

$$\begin{aligned}\|w\|^2_{\mathcal{H}(T)} \leq Ce^T\big(&\|u_0\|^2_{H^2(\Omega_i)} + \|\tilde{f}\|^2_{H^1(0,T;L^2(\Omega_i))}\\ &+\|g\|^2_{H^1(0,T;L^2(\Gamma))\cap L^\infty(0,T;H^{\frac{1}{2}}(\Gamma))}\big),\end{aligned} \tag{13}$$

where $C>0$ is a constant depending only on p and ν.

Proof. *1.* First *a priori* estimate: for w in $L^\infty(0,T;L^2(\Omega_i)) \cap L^2(0,T;H^1(\Omega_i))$.

We take the L^2 inner product of equation $w_t - \Delta w = \tilde{f}$ with w, integrate by parts in Ω_i, apply the Cauchy-Schwarz inequality and the inequality $ab \leq \frac{a^2}{\varepsilon} + \varepsilon b^2$, for $a, b \in \mathbb{R}$ and $\varepsilon \geq 0$, on the right-hand side of the resulting equation, and integrate over $[0,t]$, for $t \leq T$, to get

$$\|w(t)\|^2 + 2\nu \int_0^t \|\nabla w(s)\|^2 ds + p \int_0^t \|w(s)\|_\Gamma^2 ds \leq \|u_0\|^2 + \int_0^t \left(\|\tilde{f}(s)\|^2 + \frac{1}{p}\|g(s)\|_\Gamma^2 \right) ds + \int_0^t \|w(s)\|^2 ds.$$

Applying the Gronwall lemma yields

$$\|w\|^2_{L^\infty(0,T;L^2(\Omega_i))} + 2\nu\|\nabla w\|^2_{L^2(0,T;L^2(\Omega_i))} + p\|w\|^2_{L^2(0,T;L^2(\Gamma))} \leq e^T \big(\|u_0\|^2 + \|\tilde{f}\|^2_{L^2(0,T;L^2(\Omega_i))} + \frac{1}{p}\|g\|^2_{L^2(0,T;L^2(\Gamma))}\big). \quad (14)$$

2. Second *a priori* estimate: for w_t in $L^\infty(0,T;L^2(\Omega_i)) \cap L^2(0,T;H^1(\Omega_i))$.

We apply (14) to w_t, and we obtain

$$\|w_t\|^2_{L^\infty(0,T;L^2(\Omega_i))} + 2\nu\|\nabla w_t\|^2_{L^2(0,T;L^2(\Omega_i))} + p\|w_t\|^2_{L^2(0,T;L^2(\Gamma))} \leq e^T \big(\|w_{t0}\|^2 + \|\tilde{f}\|^2_{H^1(0,T;L^2(\Omega_i))} + \frac{1}{p}\|g\|^2_{H^1(0,T;L^2(\Gamma))}\big). \quad (15)$$

In order to estimate $\|w_{t0}\|$, we take the inner product of equation $w_t - \Delta w = \tilde{f}$ with w_t, integrate by parts in Ω_i and evaluate the resulting equation at time $t = 0$. We obtain

$$\|w_{t0}\|^2 + \nu(\nabla u_0, \nabla w_{t0}) + p(u_0, w_{t0})_\Gamma = (\tilde{f}(\cdot,0), w_{t0}) + (g(\cdot,0), w_{t0})_\Gamma.$$

Integrating by parts the second term on the left-hand side gives

$$\|w_{t0}\|^2 = \nu(\Delta u_0, w_{t0}) - (\nu\partial_{n_i} u_0, w_{t0})_\Gamma - p(u_0, w_{t0})_\Gamma + (\tilde{f}(\cdot,0), w_{t0}) + (g(\cdot,0), w_{t0})_\Gamma.$$

Since the term $-\nu\partial_{n_i} u_0 - pu_0 + g(\cdot,0)$ vanishes, we obtain, by applying the Cauchy-Schwarz inequality,

$$\|w_{t0}\| \leq \nu\|\Delta u_0\| + \|\tilde{f}(\cdot,0)\|.$$

We insert the above inequality in (15), which gives the estimate

$$\|w_t\|^2_{L^\infty(0,T;L^2(\Omega_i))} + 2\nu\|\nabla w_t\|^2_{L^2(0,T;L^2(\Omega_i))} + p\|w_t\|^2_{L^2(0,T;L^2(\Gamma))} \leq e^T \big(2\nu^2\|u_0\|^2_{H^2(\Omega_i)} + 3\|\tilde{f}\|^2_{H^1(0,T;L^2(\Omega_i))} + \frac{1}{p}\|g\|^2_{H^1(0,T;L^2(\Gamma))}\big), \quad (16)$$

3. Third *a priori* estimate: for ∇w in $L^\infty(0,T;L^2(\Omega_i))$.

We multiply the equation by w_t, use Cauchy-Schwarz lemma, to obtain

$$\|w_t\|^2_{L^2(0,T;L^2(\Omega_i))} + \nu\|\nabla w\|^2_{L^\infty(0,T;L^2(\Omega_i))} + p\|w\|^2_{L^\infty(0,T;L^2(\Gamma))} \leq \nu\|\nabla u_0\|^2 + p\|u_0\|^2_\Gamma + \|\tilde{f}\|^2_{L^2(0,T;L^2(\Omega_i))} + \frac{1}{p}\|g\|^2_{L^2(0,T;L^2(\Gamma))} + p\|w_t\|^2_{L^2(0,T;L^2(\Gamma))}. \quad (17)$$

By putting together (14), (16) and (17), we obtain by a Galerkin method, a unique solution w of (11) such that $w \in L^\infty(0,T;H^1(\Omega_i)) \cap H^1(0,T;L^2(\Omega_i)) \cap W^{1,\infty}(0,T;L^2(\Omega_i))$. It remains to get an upper bound in $L^\infty(0,T;H^2(\Omega_i))$. Since

$$\begin{cases} \Delta w = \dfrac{1}{\nu}(w_t - \tilde{f}) \in L^\infty(0,T;L^2(\Omega_i)), \\ \dfrac{\partial w}{\partial n_i} = \dfrac{1}{\nu}(g - pw) \in L^\infty(0,T;H^{1/2}(\Gamma)), \end{cases}$$

classical regularity results prove that $w \in L^\infty(0,T;H^2(\Omega_i))$ with

$$\begin{aligned} \|w\|_{L^\infty(0,T;H^2(\Omega_i))} &\leq C_1(\|\Delta w\|_{L^\infty(0,T;L^2(\Omega_i))} + \|\frac{\partial w}{\partial n_i}\|_{L^\infty(0,T;H^{1/2}(\Gamma))}), \\ &\leq C_2(\|w_t\|_{L^\infty(0,T;L^2(\Omega_i))} + \|\tilde{f}\|_{L^\infty(0,T;L^2(\Omega_i))} \\ &\qquad + \|g\|_{L^\infty(0,T;H^{\frac{1}{2}}(\Gamma))} + \|w\|_{L^\infty(0,T;H^1(\Omega_i))}). \end{aligned} \tag{18}$$

We deduce then that problem (11) has a unique solution w in $\mathcal{H}(T)$, which satisfies (13). □

In order to estimate the nonlinear terms, we will use use the regularity of f.

Lemma 3.2. *Let $\mathcal{O}$ be a regular domain in $\mathbb{R}^2$, F a $\mathcal{C}^1$ real function. There exists a continuous positive increasing function φ such that, for any v and w in $H^2(\mathcal{O})$,*

$$\|F(w) - F(v)\|_{L^2(\mathcal{O})} \leq \varphi(max(\|w\|_\infty, \|v\|_\infty))\|w - v\|_{L^2(\mathcal{O})}. \tag{19}$$

The function φ is given by

$$\varphi(a) = \sup_{|\xi| \in (0,a)} |F'(\xi)|.$$

Proof. Note first that $H^2(\mathcal{O})$ is a subset of $L^\infty(\mathcal{O})$ with continuous injection, which gives a meaning to (19). We use now the Mean Value Theorem. For any a, b in $\mathbb{R}$,

$$|F(a) - F(b)| = \left| \int_a^b F'(\xi) d\xi \right| \leq |a - b| \sup_{\xi \in (a,b)} |F'(\xi)|.$$

We apply the above inequality to the functions w and v,

$$|F(w(x)) - F(v(x))| \leq |w(x) - v(x)| \sup_{|\xi| \in (0, max(\|v\|_\infty, \|w\|_\infty))} |F'(\xi)|.$$

The function

$$\varphi : a \to \sup_{|\xi| \in (0,a)} |F'(\xi)|$$

is an increasing function over $\mathbb{R}^+$, which finishes the proof of the lemma. □

We now define the map which will be used for the definition of the nonlinear problem.

Lemma and definition 3.3. Let $T > 0$. Let $u_0 \in H^2(\Omega_i)$, $g \in H^1(0,T;L^2(\Gamma)) \cap L^\infty(0,T;H^{\frac{1}{2}}(\Gamma))$. For any $v \in \mathcal{H}(T)$, the linear problem

$$\begin{cases} w_t - \nu \Delta w = -f(v), & \text{in } \Omega_i \times (0,T), \\ w(\cdot,\cdot,0) = u_{0|\Omega_i}, & \text{in } \Omega_i, \\ \nu \frac{\partial w}{\partial n_i} + pw = g, & \text{over } \Gamma \times (0,T). \end{cases} \tag{20}$$

has a unique solution in $\mathcal{H}(T)$, hence defining an application $w = \mathcal{T}(v)$ in $\mathcal{H}(T)$, with

$$\begin{aligned}\|\mathcal{T}(v)\|^2_{\mathcal{H}(T)} \le Ce^T\big(\|u_0\|^2_{H^2(\Omega_i)} + \|g\|^2_{H^1(0,T;L^2(\Gamma))\cap L^\infty(0,T;H^{\frac12}(\Gamma))} \\ +T(\varphi(\|v\|_{L^\infty((0,T)\times\Omega_i)}))^2\|v\|^2_{W^{1,\infty}(0,T;L^2(\Omega_i))}\big)\end{aligned} \tag{21}$$

Proof. Since $f(0) = 0$, we have by Lemma 3.2,

$$\|f(v)\|_{L^2(0,T;L^2(\Omega_i))} \le \sqrt{T}\varphi(\|v\|_{L^\infty((0,T)\times\Omega_i)})\|v\|_{L^\infty(0,T;L^2(\Omega_i))}.$$

On another hand, we have by the definition of φ:

$$\|f'(v)v_t\|_{L^2(0,T;L^2(\Omega_i))} \le \sqrt{T}\varphi(\|v\|_{L^\infty((0,T)\times\Omega_i)})\|v\|_{L^\infty(0,T;L^2(\Omega_i))}.$$

These inequalities finally give that $f(v)$ is in $H^1(0,T;L^2(\Omega_i))$, and

$$\|f(v)\|_{H^1(0,T;L^2(\Omega_i))} \le \sqrt{T}\varphi(\|v\|_{L^\infty((0,T)\times\Omega_i)})\|v\|_{W^{1,\infty}(0,T;L^2(\Omega_i))}. \tag{22}$$

By Lemma 3.1, we conclude that the linear problem (20) has a unique solution w in $\mathcal{H}(T)$, and the estimate comes directly from (13).

□

Let M be such that

$$M^2 \ge 4C(\|u_0\|^2_{H^2(\Omega_i)} + \|g\|^2_{H^1(0,T;L^2(\Gamma))\cap L^\infty(0,T;H^{\frac12}(\Gamma))}), \tag{23}$$

where C is the universal constant of estimate (21), and define the time

$$T_0(M) = \sup\{T' \le T, \quad \max\big(\frac{e^{T'}}{2},\ 2Ce^{T'}(\varphi(M))^2T',\ 2e^{\frac{T'}{2}}\sqrt{T'}\varphi(M)\big) \le 1\}. \tag{24}$$

Lemma 3.4. *Define*

$$\mathcal{B}_M := \{w \in \mathcal{H}(T_0)\ :\ \|w\|_{\mathcal{H}(T_0)} \le M\}.$$

Then $\mathcal{T}(\mathcal{B}_M) \subseteq \mathcal{B}_M$.

Proof. If $v \in \mathcal{B}_M$, $\|v\|_{W^{1,\infty}((0,T)\times\Omega_i)} \le M$, and since φ is increasing, we deduce from (21) that

$$\begin{aligned}\|\mathcal{T}(v)\|^2_{\mathcal{H}(T_0)} &\le Ce^{T_0}(\|u_0\|^2_{H^2(\Omega_i)} + T_0(M\varphi(M))^2 + \|g\|^2_{H^1(0,T_0;L^2(\Gamma))\cap L^\infty(0,T_0;H^{\frac12}(\Gamma))}), \\ &\le M^2(\frac14 e^{T_0} + CT_0e^{T_0}(\varphi(M))^2), \\ &\le M^2 \text{ by definition of } T_0.\end{aligned}$$

□

Lemma 3.5. *$\mathcal{B}_M$ is a closed metric subspace of $L^\infty(0,T_0;L^2(\Omega_i))$, and $\mathcal{T}$ is a contraction in $\mathcal{B}_M$.*

Proof. We first prove that B_M is closed in $L^\infty(0,T_0;L^2(\Omega_i))$. Indeed let $(w_n)_{n\in\mathbb{N}}$ be a sequence in $\mathcal{B}_M$ converging to w in $L^\infty(0,T_0;L^2(\Omega_i))$. Since $\mathcal{B}_M$ is weakly compact in $\mathcal{H}(T_0)$, there exists a subsequence $w_{n'}$ converging weakly to $\tilde{w} \in \mathcal{B}_M$ in $\mathcal{H}(T_0)$. By the uniqueness of the weak limit, $w = \tilde{w}$ and thus $w \in \mathcal{B}_M$.

Let v and $\bar{v} \in \mathcal{B}_M$ and put $w = \mathcal{T}(v),\ \bar{w} = \mathcal{T}(\bar{v})$. We have that $w - \bar{w}$ satisfies

$$\begin{cases}(w-\bar{w})_t - \nu\Delta(w-\bar{w}) = -(f(v)-f(\bar{v})), & \text{in } \Omega_i\times(0,T_0),\\ (w-\bar{w})(\cdot,0) = 0, & \text{in } \Omega_i,\\ \nu\frac{\partial}{\partial n}(w-\bar{w}) + p(w-\bar{w}) = 0, & \text{over } \Gamma\times(0,T_0).\end{cases} \tag{25}$$

By taking the inner product of the first equation in the system above with $w - \bar{w}$, integrating by parts and applying the Cauchy-Schwarz inequality and inequality $ab \leq \frac{a^2}{2} + \frac{b^2}{2}$, $a, b \in \mathbb{R}$, on the right-hand side, we obtain

$$\frac{1}{2}\frac{d}{dt}\|w-\bar{w}\|^2 + \nu\|\nabla(w-\bar{w})\|^2 + p\|w-\bar{w}\|_\Gamma^2 \leq \frac{1}{2}(\|f(v)-f(\bar{v})\|^2 + \|w-\bar{w}\|^2).$$

We integrate the above inequality over $[0,t]$, for $t \leq T_0$, and we apply the Gronwall lemma to obtain

$$\|(w-\bar{w})(t)\|^2 \leq e^t \int_0^t \|f(v(s)) - f(\bar{v}(s))\|^2 ds.$$

Again by Lemma 3.2, we have

$$\|(w-\bar{w})\|^2_{L^\infty(0,T_0;L^2(\Omega_i))} \leq e^{T_0} T_0 (\varphi(M))^2 \|v-\bar{v}\|^2_{L^\infty(0,T_0;L^2(\Omega_i))},$$

and by the definition of T_0, we conclude that

$$\|(w-\bar{w})\|_{L^\infty(0,T_0;L^2(\Omega_i))} \leq \frac{1}{2}\|(v-\bar{v})\|_{L^\infty(0,T_0;L^2(\Omega_i))}, \tag{26}$$

which proves the result. □

By the Picard theorem, the map $\mathcal{T}$ has a unique fixed point in $\mathcal{B}_M$, which proves the existence and uniqueness of a solution $w \in \mathcal{B}_M$ to the nonlinear problem. Furthermore, we have for $i \in \{1,2\}$ and $j = 3 - i$,

$$B_j(w) := -\nu\frac{\partial w}{\partial n_i} + pw = -g + 2pw \in H^1(0,T_0;L^2(\Gamma)) \cap L^\infty(0,T_0;H^{\frac{1}{2}}(\Gamma)). \tag{27}$$

We are now able to give a precise meaning to the algorithm. To simplify the notations, we set $V_\Gamma(T) = H^1(0,T;L^2(\Gamma)) \cap L^\infty(0,T;H^{\frac{1}{2}}(\Gamma))$. Let (g_1^0, g_2^0) in $(V_\Gamma(T))^2$, and

$$M_0^2 \geq 4C(\|u_0\|^2_{H^2(\Omega_i)} + \|g_i^0\|^2_{V_\Gamma(T_0)}).$$

By Lemma 3.5, we can define (u_1^0, u_2^0) in $(\mathcal{H}(T_0))^2$ and, by (27), $(g_1^1, g_2^1) = (B_1 u_2^0, B_2 u_1^0) \in (V_\Gamma(T_0))^2$. We thus build a sequence of numbers M_k such that

$$M_k^2 \geq 4C(\|u_0\|^2_{H^2} + \|B_i(u_j^{k-1})\|^2_{V_\Gamma(T_{k-1})}),$$

and a decreasing sequence of times $T_k = T(M_k)$ such that (u_1^k, u_2^k) is defined in $\mathcal{H}(T_k)$.

3.2. **Proof of theorem 2.3.**

For each $k > 0$, we define the errors $e_i^k = u_i^k - u_{|\Omega_i}$, which satisfy the equations

$$\begin{cases} \partial_t e_i^k - \nu\Delta e_i^k = -f(u_i^k) + f(u), & \text{in } \Omega_i \times [0,T_k), \\ e_i^k(\cdot,\cdot,0) = 0, & \text{in } \Omega_i, \\ \nu\dfrac{\partial e_i^k}{\partial n_i} + pe_i^k = \nu\dfrac{\partial e_j^{k-1}}{\partial n_i} + pe_j^{k-1}, & \text{over } \Gamma \times [0,T_k), \end{cases}$$

where $i \in \{1,2\}$ and $j = 3 - i$.

By taking the inner product of equation $\partial_t e_i^k - \nu\Delta e_i^k = -f(u_i^k) + f(u)$ with e_i^k, by integrating by parts in Ω_i, we obtain

$$\frac{1}{2}\frac{d}{dt}\|e_i^k\|^2 + \nu\|\nabla e_i^k\|^2 - \nu\Big(\frac{\partial e_i^k}{\partial n_i}, e_i^k\Big)_\Gamma = (f(u) - f(u_i^k),\, e_i^k).$$

By using Cauchy-Schwarz inequality and Lemma 3.2, we obtain

$$\frac{1}{2}\frac{d}{dt}\|e_i^k\|^2 + \nu\|\nabla e_i^k\|^2 - \nu\Big(\frac{\partial e_i^k}{\partial n_i}, e_i^k\Big)_\Gamma \le \varphi(\|u_i^k(t)\|_\infty)\|e_i^k\|^2.$$

Note that we have omitted the dependence of φ with respect to u. We now replace the boundary term (an argument discovered by Després in [1]) using the identity

$$\nu\Big(\frac{\partial e_i^k}{\partial n_i}, e_i^k\Big)_\Gamma = \frac{1}{4p}\Big\{\Big\|\nu\frac{\partial e_i^k}{\partial n_i} + pe_i^k\Big\|_\Gamma^2 - \Big\|\nu\frac{\partial e_i^k}{\partial n_i} - pe_i^k\Big\|_\Gamma^2\Big\}.$$

Hence,

$$\frac{1}{2}\frac{d}{dt}\|e_i^k\|^2 + \nu\|\nabla e_i^k\|^2 + \frac{1}{4p}\Big\|\nu\frac{\partial e_i^k}{\partial n_i} - pe_i^k\Big\|_\Gamma^2 \le \varphi(\|u_i^k(t)\|_\infty)\|e_i^k\|^2 + \frac{1}{4p}\Big\|\nu\frac{\partial e_i^k}{\partial n_i} + pe_i^k\Big\|_\Gamma^2. \quad (28)$$

We add now (28) for $i = 1, 2$ and use the transmission condition on the right-hand side of the resulting equation. Defining

$$E(w)(t) = \frac{1}{2}\|w(t)\|^2 + \nu\int_0^t \|\nabla w(s)\|^2 ds,$$

and the boundary errors

$$\tilde{g}_i^k = \nu\frac{\partial e_i^k}{\partial n_i} - pe_i^k, \quad (29)$$

we obtain

$$\begin{aligned}\frac{d}{dt}\big(E(e_1^k)(t) + E(e_2^k)(t)\big) + \frac{1}{4p}(\|\tilde{g}_1^k\|_\Gamma^2 + \|\tilde{g}_2^k\|_\Gamma^2) \le \\ \frac{1}{4p}(\|\tilde{g}_1^{k-1}\|_\Gamma^2 + \|\tilde{g}_2^{k-1}\|_\Gamma^2) \\ +\varphi(\|u_1^k(t)\|_\infty)\|e_1^k\|^2 + \varphi(\|u_2^k(t)\|_\infty)\|e_2^k\|^2.\end{aligned} \quad (30)$$

We differentiate now equation $\partial_t e_i^k - \nu\Delta e_i^k = -f(u_i^k) + f(u)$ with respect to t, take the inner product of the resulting equation with $\partial_t e_i^k$, and integrate by parts in Ω. We can write the right-hand side of the resulting equation as

$$\begin{aligned}(\partial_t(f(u) - f(u_i^k)), \partial_t e_i^k) &= (f'(u)\partial_t u - f'(u_i^k)\partial_t u + f'(u_i^k)\partial_t u - f'(u_i^k)\partial_t u_i^k, \partial_t e_i^k) \\ &= ((f'(u) - f'(u_i^k))\partial_t u, \partial_t e_i^k) - (f'(u_i^k)\partial_t e_i^k, \partial_t e_i^k). \quad (31)\end{aligned}$$

We again use Lemma 3.2 for f' with a new function φ_1. If we apply now the Cauchy-Schwarz inequality and inequality $ab \le \frac{a^2}{2} + \frac{b^2}{2}$, we get

$$\begin{aligned}&(\partial_t(f(u_i^k) - f(u)), \partial_t e_i^k) \\ &\quad\le \varphi(\|u_i^k(t)\|_\infty)\|\partial_t e_i^k\|^2 + \frac{1}{2}\varphi_1(\|u_i^k(t)\|_\infty)\|\partial_t u\|_{L^\infty(0,T;L^2)}(\|\partial_t e_i^k\|^2 + \|e_i^k\|^2).\end{aligned}$$

We introduce $\varphi_2 = \varphi + \frac{1}{2}\|\partial_t u\|_{L^\infty(0,T;L^2)}\varphi_1$ which is also continuous positive increasing, and end up with

$$\frac{1}{2}\frac{d}{dt}\|\partial_t e_i^k\|^2 + \nu\|\partial_t\nabla e_i^k\|^2 - \Big(\nu\frac{\partial}{\partial n_i}\partial_t e_i^k, \partial_t e_i^k\Big)_\Gamma \le \varphi_2(\|u_i^k\|_\infty)(\|\partial_t e_i^k\|^2 + \|e_i^k\|^2). \quad (32)$$

We now add equations (32) for $i = 1, 2$, use the derivative in time of the transmission condition, and proceed as before. We obtain

$$\begin{aligned}\frac{d}{dt}\big(E(\partial_t e_1^k)(t) + E(\partial_t e_2^k)(t)\big) + \frac{1}{4p}(\|\partial_t \tilde{g}_1^k\|_\Gamma^2 + \|\partial_t \tilde{g}_2^k\|_\Gamma^2) \le \\ \frac{1}{4p}(\|\partial_t \tilde{g}_1^{k-1}\|_\Gamma^2 + \|\partial_t \tilde{g}_2^{k-1}\|_\Gamma^2) \\ +\varphi_2(\|u_1^k(t)\|_\infty)\|\partial_t e_1^k\|^2 + \varphi_2(\|u_2^k(t)\|_\infty)\|\partial_t e_2^k\|^2.\end{aligned} \tag{33}$$

We finally perform the same calculation on the derivatives in the y direction.

$$\begin{aligned}\frac{d}{dt}\big(E(\partial_y e_1^k)(t) + E(\partial_y e_2^k)(t)\big) + \frac{1}{4p}(\|\partial_y \tilde{g}_1^k\|_\Gamma^2 + \|\partial_y \tilde{g}_2^k\|_\Gamma^2) \le \\ \frac{1}{4p}(\|\partial_y \tilde{g}_1^{k-1}\|_\Gamma^2 + \|\partial_y \tilde{g}_2^{k-1}\|_\Gamma^2) \\ +\varphi_3(\|u_1^k(t)\|_\infty)\|\partial_y e_1^k\|^2 + \varphi_3(\|u_2^k(t)\|_\infty)\|\partial_y e_2^k\|^2.\end{aligned} \tag{34}$$

We now define the total energy in the domains at step k as a function of time t to be

$$\mathcal{E}^k := \sum_1^2 (E(e_i^k) + E(\partial_t e_i^k) + E(\partial_y e_i^k)),$$

and the total boundary error at step k as a function of time t to be

$$\mathcal{G}_i^k := \frac{1}{4p}\big(\|\tilde{g}_i^k\|_\Gamma^2 + \|\partial_t \tilde{g}_i^k\|_\Gamma^2 + \|\partial_y \tilde{g}_1^k\|_\Gamma^2\big),$$
$$\mathcal{G}^k = \mathcal{G}_1^k + \mathcal{G}_2^k.$$

If we add (30) to (33) and (34), we obtain

$$\frac{d}{dt}\big(\mathcal{E}^k(t)\big) + \mathcal{G}^k(t) \le \big(\varphi_4(\|u_1^k\|_\infty) + \varphi_4(\|u_2^k\|_\infty)\big)\mathcal{E}^k(t) + \mathcal{G}^{k-1}(t). \tag{35}$$

Let

$$\mathcal{E}_S^K = \sum_{k=0}^K \mathcal{E}^k, \quad \mathcal{U}^K(t) = \sup_{0\le k\le K}\|u_1^k(t)\|_\infty + \sup_{0\le k\le K}\|u_2^k(t)\|_\infty.$$

We sum both sides of (35) over $k = 0, \cdots, K$, and integrate on $(0, T)$. Since $\mathcal{E}_S^K(0) = 0$, we obtain for a new function φ_5:

$$\left\{\begin{array}{lcl} \mathcal{E}_S^K(t) + \int_0^t \mathcal{G}^K(s)ds & \le & 2\int_0^t \varphi_5\big(\mathcal{U}^K(s)\big)\mathcal{E}_S^K(s)ds + \int_0^t \mathcal{G}^0(s)ds, \\ \max_{0\le k\le K}\int_0^t \mathcal{G}^k(s)ds & \le & 2\int_0^t \varphi_5\big(\mathcal{U}^K(s)\big)\mathcal{E}_S^K(s)ds + \int_0^t \mathcal{G}^0(s)ds. \end{array}\right. \tag{36}$$

We now estimate $\mathcal{U}^K$. We have for $i = 1, 2$ and $0 \le k \le K$:

$$\|u_i^k(t)\|_\infty \le \|u(t)\|_\infty + \|e_i^k(t)\|_\infty.$$

The norm of $e_i^k(t)$ in $L^\infty(\Omega_i)$ is bounded by $C_2\|e_i^k(t)\|_{H^2(\Omega_i)}$, which can be estimated as in (18), and gives

$$\|u_i^k(t)\|_\infty \le C_3(1 + \|\partial_t e_i^k(t)\| + \|f(u_i^k(t)) - f(u(t))\| + \|\tilde{g}_i^k(t)\|_{H^{\frac{1}{2}}(\Gamma)}).$$

We now estimate $\|g\|_{L^\infty(0,t;H^{\frac{1}{2}}(\Gamma))}$:

$$\begin{aligned}\|g\|^2_{L^\infty(0,t;H^{\frac{1}{2}}(\Gamma))} &\leq 2\|g\|_{L^2(0,t;H^1(\Gamma))}\|\partial_t g\|_{L^2(0,t;L^2(\Gamma))}\\ &\leq \|g\|^2_{H^1((0,t)\times\Gamma)}.\end{aligned}$$

We can rewrite

$$\begin{aligned}\|u_i^k(t)\|_\infty &\leq C_4(1+\|\partial_t e_i^k(t)\|+\|f(u_i^k(t))-f(u(t))\|+\|\tilde{g}_i^k\|_{H^1((0,t)\times\Gamma)})\\ &\leq C_4(4+2\mathcal{E}^k(t)+(\varphi(\|u_i^k(t)\|_\infty))^2\mathcal{E}^k(t)+\int_0^t \mathcal{G}^k(s)\,ds),\end{aligned}$$

where $\|u\|_{L^\infty((0,T)\times\Omega)}$ has been included in the constant C_4. This yields for $\mathcal{U}^K$ the estimate:

$$\mathcal{U}^K(t)\leq 4C_4(1+\mathcal{E}_S^K(t)+(\varphi(\mathcal{U}^K(t)))^2\mathcal{E}_S^K(t)+\max_{0\leq k\leq K}\int_0^t \mathcal{G}^k(s)\,ds). \tag{37}$$

The functions $t\to\mathcal{E}_S^k(t)$ and $t\to\mathcal{U}^k(t)$ are continuous. We fix M such that

$$M\leq \frac{1}{4(2+(\varphi(5C_4))^2)}\ ,$$

and define

$$\overline{T}=\inf\{T'\leq T_0(M),\quad 2T'\varphi_5(5C_4)M+\int_0^{T'}\mathcal{G}^0(s)ds\geq M\},$$

$$\underline{T}=\sup\{T',\quad \mathcal{E}_S^K\leq M \text{ and } \mathcal{U}^K\leq 5C_4 \text{ on } (0,T')\}.$$

By continuity, we have either $\mathcal{E}_S^K(\underline{T})=M$ or $\mathcal{U}^K(\underline{T})=5C_4$. In the first case we have by (36),

$$M=\mathcal{E}_S^K(\underline{T})\leq 2M\underline{T}\varphi_5(5C_4)+\int_0^{\underline{T}}\mathcal{G}^0(s)ds,$$

which implies that $\underline{T}\geq\overline{T}$. In the second case we have by (36) and (37),

$$5C_4=\mathcal{U}^K(\underline{T})\leq 4C_4(1+[(\varphi(5C_4))^2+2](2M\underline{T}\varphi_5(5C_4)+\int_0^{\underline{T}}\mathcal{G}^0(s)ds)).$$

This can be rewritten as

$$2\underline{T}\varphi_5(5C_4)M+\int_0^{\underline{T}}\mathcal{G}^0(s)ds\geq\frac{1}{4(2+(\varphi(5C_4))^2)}\quad .$$

By the assumption on M, this implies that

$$2\underline{T}\varphi_5(5C_4)M+\int_0^{\underline{T}}\mathcal{G}^0(s)ds\geq M,$$

and therefore $\underline{T}\geq\overline{T}$. We thus have

$$\forall t\in(0,\overline{T}),\mathcal{E}_S^K(t)\leq M,\quad \int_0^t\mathcal{G}_M^K(s)ds\leq M,\quad \mathcal{U}^K(t)\leq 5C_4. \tag{38}$$

Suppose now the initial data to be such that

$$\|u_0\|^2_{H^2(\Omega_i)}+\|g_i^0\|^2_{H^1(0,\overline{T};L^2(\Gamma))\cap L^\infty(0,\overline{T};H^{\frac{1}{2}}(\Gamma))}\leq\frac{M^2}{4C}.$$

The local existence of the u_i^k is ensured by Theorem 2.2, and by the previous analysis, a classical compactness argument proves that they all have a time of existence at least equal to $\overline{T}$.

3.3. **Proof of theorem 2.4.** We deduce from (38) that the infinite series with general term $\mathcal{E}^k$ converges in $L^\infty(0,\overline{T})$. Therefore the general term tends to zero and u_i^k converges to $u_{|\Omega_i}$ in $L^\infty(0,\overline{T};H^1(\Omega_i))$.

4. **The numerical treatment of the algorithm.** We describe in this section the numerical discretization of the initial and boundary value subdomain problems and the numerical implementation of the iterative SWR algorithm. We discretize the subdomain problems by finite elements in space and a finite difference discretization in time, implicit for the linear part and explicit for the nonlinear term.

4.1. **The best choice for the transmission conditions.** The efficiency of the linear Robin and second order transmission conditions defined by the operators (6) and (7) is attained by a careful choice of the constants p and q. In [2] and in [6], asymptotic formulas (in Δt) for the values of p and q, that optimize the convergence factor of the algorithm, were written. These results are based on Fourier transforms in time and in the transverse direction y of the error equations. For the linear reaction-diffusion equation

$$\partial_t u - \nu \Delta u + bu = 0,$$

where b is a positive constant, explicit formulas for the optimal parameters are given. In the case of Robin transmission conditions, we obtain

$$p_{opt}^R(\Delta t, b, \nu) = \frac{\sqrt{\pi\nu}\big(2\sqrt{(4\nu b + 4\nu^2 {k_m}^2)^2 + 16\nu^2 w_m} + 4\nu b + 4\nu^2 {k_m}^2\big)^{\frac{1}{4}}}{\Delta t^{\frac{1}{2}}}, \tag{39}$$

where $k_m = \frac{\pi}{L}$ and $w_m = \frac{\pi}{2T}$, L being the domain decomposition interface length and T the time interval length (see [5] and [6]) ; in the case of order 2 transmission conditions, we obtain more complicated formulas

$$(p_{opt}^V, q_{opt}^V)(\Delta t, b, \nu), \tag{40}$$

which are detailed in [2] (cf. p. 212).

Such an analysis is essentially linear. However, the equation satisfied by the errors $e_i^k = u_i^k - u$ is

$$\partial_t e_i^k - \nu \nabla e_i^k + f(u_i^k) - f(u) = 0,$$

and a linearization around u_i^k gives

$$\partial_t e_i^k - \nu \nabla e_i^k + f'(u_i^k) e_i^k \simeq 0.$$

Therefore the best parameters can be used in two ways.

(i) By using linear transmission operators with values corresponding to expected values of $f'(u)$,

(ii) by introducing nonlinear transmission conditions, where b is chosen to be $f'(u_i^k)$ in the formulas (39) for Robin, and (40) for second order transmission conditions.

No well-posedness analysis is available for the algorithm with nonlinear transmission conditions. We present however, in section 5, numerical results which illustrate the convergence of the numerical approximation of this nonlinear algorithm.

4.2. **Discretization scheme.** We consider here a bounded domain Ω in $\mathbb{R}^2$, homogeneous Dirichlet boundary data are imposed on the boundary $\partial\Omega$ of Ω. It is divided into two nonoverlapping subdomains Ω_j, and the common boundary Γ is supposed to meet $\partial\Omega$ orthogonally, see Figure 1. This assumption is essential only for the second order transmission condition, and permits to extend the analysis in Section 2.

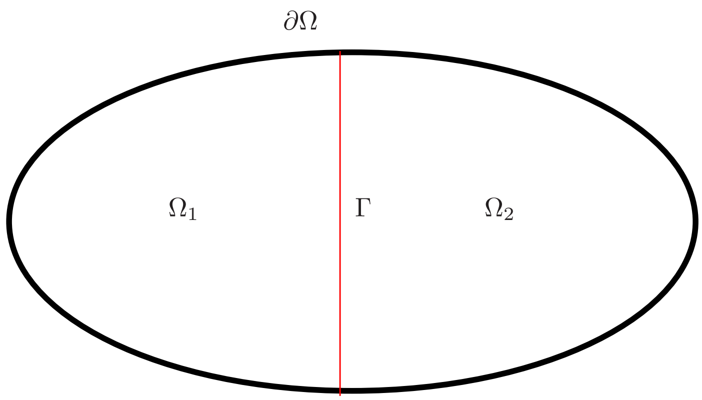

FIGURE 1. Decomposition in subdomains $\overline{\Omega} = \overline{\Omega}_1 \cup \overline{\Omega}_2$

Let us first describe the numerical method in the case of linear Robin or second order boundary operators. The first task is the discretization of the boundary value problem (8), in $V_0 = \{v \in V, \quad v = 0 \text{ on } \partial\Omega \cap \partial\Omega_i\}$.

We consider V_h, a finite dimensional subspace of V of piecewise $\mathbb{P}_1$ functions, and a basis $\varphi_1, \dots, \varphi_I$ of V_h, $S_1, \dots, S_I$ being the vertices of the triangulation. We search an approximate solution

$$u_h(t) = u_1(t)\varphi_1 + \cdots + u_I(t)\varphi_I,$$

which satisfies

$$(u_h', \varphi_i) + +\nu(\nabla u_h, \nabla\varphi_i) + p(u_h, \varphi_i)_\Gamma + q(u_h', \varphi_i)_\Gamma \\ + \nu q(\frac{\partial u_h}{\partial y}, \frac{\partial \varphi_i}{\partial y})_\Gamma + (f(u_h), \varphi_i) = (g, \varphi_i)_\Gamma, \; i = 1, \dots, I.$$

Denote by $t^n = n\Delta t$ the time grid points for $0 \le n \le N$, and let $u^n = u_1^n\varphi_1 + \cdots + u_I^n\varphi_I$ be the approximate solution at time t^n. We use a linearly implicit Euler scheme: if the approximate numerical solution $U^n = (u_1^n, \cdots, u_I^n)$ at time t^n is given, the solution U^{n+1} at time t^{n+1} is computed by solving the algebraic system

$$\Big(\frac{1}{\Delta t}(M + qM_\Gamma) + \nu K + pM_\Gamma + \nu q K_\Gamma\Big)U^{n+1} = \\ \frac{1}{\Delta t}(M + qM_\Gamma)U^n - MF(U^n) + M_\Gamma G^{n+1}, \quad (41)$$

where the mass and stiffness matrices are defined by $M_{i,j} = (\varphi_j, \varphi_i)$ and $K_{i,j} = (\nabla\varphi_j, \nabla\varphi_i)$, and on the boundary $M_{\Gamma i,j} = (\varphi_j, \varphi_i)_\Gamma$ and $K_{\Gamma i,j} = (\partial_y\varphi_j, \partial_y\varphi_i)$. We set $F(U^n) = (f(u_1^n), \dots, f(u_I^n))$ and $G^{n+1} = \big(g(S_1, t^{n+1}), \cdots, g(S_I, t^{n+1})\big)$.

Considering nonlinear transmission conditions leads to the discretization of the boundary value problem (8), where in the linear operators (6) and (7), the constants p and (p, q) are replaced by nonlinear functions $p(u) = p^R_{opt}(\Delta t, f'(u), \nu)$ and

$(p,q)(u) = (p^V_{opt}, q^V_{opt})(\Delta t, f'(u), \nu)$, in such a way that the third equation of (8) is replaced by

$$\nu \frac{\partial u}{\partial n_i} + p(u)u + q(u)(\frac{\partial u}{\partial t} - \nu \frac{\partial^2 u}{\partial y^2}) = g.$$

In this case the coefficients p and q are replaced by the time-dependent matrices

$$\mathrm{Diag}^n_p = \mathrm{diag}(p(u^n_1), \ldots, p(u^n_I)), \quad \mathrm{Diag}^n_q = \mathrm{diag}(q(u^n_1), \ldots, q(u^n_I)).$$

The linear system (41) is solved with the LU procedure.

4.3. **Implementation of the iterative algorithm.** A step of the iterative Schwarz waveform relaxation algorithm consists in solving the initial and boundary value problems in each subdomain and in defining the new boundary conditions for the next step. We therefore have to discretize the operator

$$(u^k_1, u^k_2) \longrightarrow (B_1(u^k_2), B_2(u^k_1)).$$

To do so, we remark that, if at step k of the algorithm, the transmission conditions are defined by

$$\nu \frac{\partial u^k_i}{\partial n_i} + p(u^k_i)u^k_i + q(u^k_i)(\frac{\partial u^k_i}{\partial t} - \nu \frac{\partial^2 u^k_i}{\partial y^2}) = g^k_i, \tag{42}$$

$i = 1, 2$, (with the possibility to take into account constant functions $p(u)$ and $q(u)$ or $q(u) = 0$), at step $k+1$, the transmission conditions are defined by (42), with

$$\begin{aligned} g^{k+1}_i =& \nu \frac{\partial u^k_j}{\partial n_i} + p(u^k_j)u^k_j + q(u^k_j)(\frac{\partial u^k_j}{\partial t} - \nu \frac{\partial^2 u^k_j}{\partial y^2}) \\ =& -\Big(\nu \frac{\partial u^k_j}{\partial n_j} + p(u^k_j)u^k_j + q(u^k_j)(\frac{\partial u^k_j}{\partial t} - \nu \frac{\partial^2 u^k_j}{\partial y^2})\Big) \\ & + 2p(u^k_j)u^k_j + 2q(u^k_j)(\frac{\partial u^k_j}{\partial t} - \nu \frac{\partial^2 u^k_j}{\partial y^2}) \\ =& -g^k_j + 2p(u^k_j)u^k_j + 2q(u^k_j)(\frac{\partial u^k_j}{\partial t} - \nu \frac{\partial^2 u^k_j}{\partial y^2}), \end{aligned}$$

with $i = 1,\ j = 2$ or $i = 2,\ j = 1$. Rewriting the transmission condition in this way has the advantage that no normal derivative has to be computed (cf. [7] for further details on this kind of technique). We discretize then the boundary condition g^k_i by considering the discretizations of the corresponding terms defined in the previous paragraphs.

5. **Numerical results.** In this section, the spatial domain is the square $\Omega = (-1, 1) \times (0, 2)$, decomposed into two subdomains $\Omega_1 = (-1, 0) \times (0, 2)$ and $\Omega_2 = (0, 1) \times (0, 2)$. The diffusion coefficient ν is equal to 1. We test here the nonlinear functions $f(u) = u^3$ and $f(u) = 10(e^u - 1)$ on the time interval $(0, 1)$. We compare in the next figures the results obtained with the linear and nonlinear Robin and second order transmission conditions described in the previous sections. The figures represent the error between the domain decomposition solution obtained after a fixed number of iterations, and the so-called mono-domain solution, which corresponds to the numerical solution computed in the global domain Ω, by using the same discretization. The boundary conditions at the boundary $\partial\Omega$ are of Dirichlet type. We considered constant initial data and three spatial meshes, corresponding to the values of $h = 0.125,\ h = 0.0625$ and $h = 0.03125$ The time step Δt is such that $\Delta t = h$.

Figure 2 illustrates the case where $f(u) = u^3$. We draw the convergence history for the algorithm with linear transmission, with the optimal parameters computed for the heat equation. On the same figure we draw the convergence history for the nonlinear transmission. These figures show first that both strategy are relevant and give linear convergence as in the linear case, although no analysis exists at the moment for the nonlinear equation. Second that the Ventcell transmission conditions perform remarkably well, and are quite insensitive to mesh refinement. The comparison also shows that the behaviors are very similar: in fact for this test case, $f'(u)$ remains small, therefore the use of the linear parameter seems to be relevant.

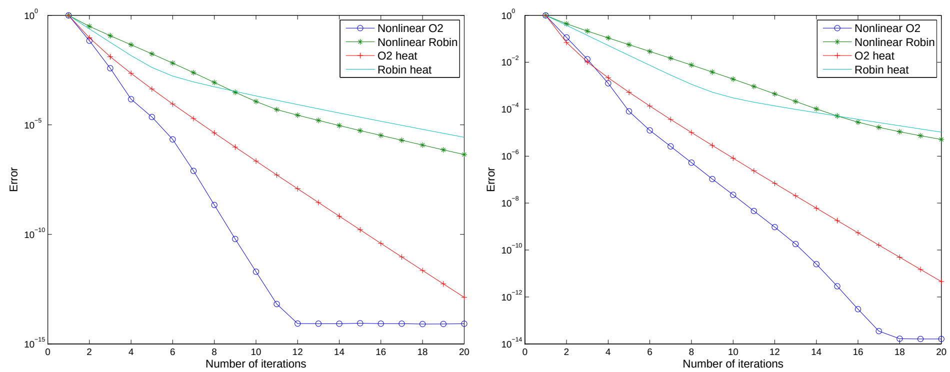

FIGURE 2. For $f(u) = u^3$, error history in $L^\infty(0,T;L^2(\Omega))$. On the left, $h = 0.0625$, an on the right $h = 0.03125$.

In Figures 3 and 4 we turn to $f(u) = 10(e^u - 1)$. We first perform in Figure 3 the same computations as before, with the coefficients inherited from the heat equation, and with the nonlinear coefficients. We see the same properties, but one more information: the linear conditions perform poorly when the behavior of $f'(u)$ cannot be anticipated.

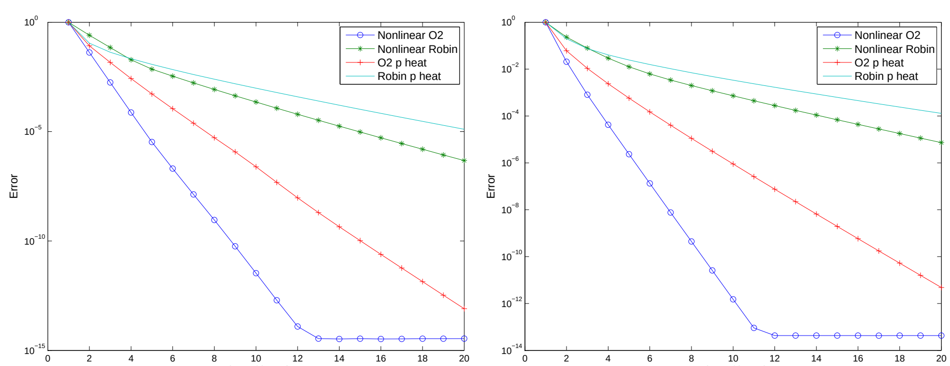

FIGURE 3. For $f(u) = 10(e^u - 1)$, error history in $L^\infty(0,T;L^2(\Omega))$. On the left, $h = 0.0625$, an on the right $h = 0.03125$.

If we know that u is quite small on the interface, thus that $f'(u)$ is close to 10, we can use the parameters p and (p, q) obtained by taking $b = 10$ in formulas (39) and (40). The situation returns now to the previous case: the linear and nonlinear strategy produce similar convergence curves, as demonstrated in Figure 4.

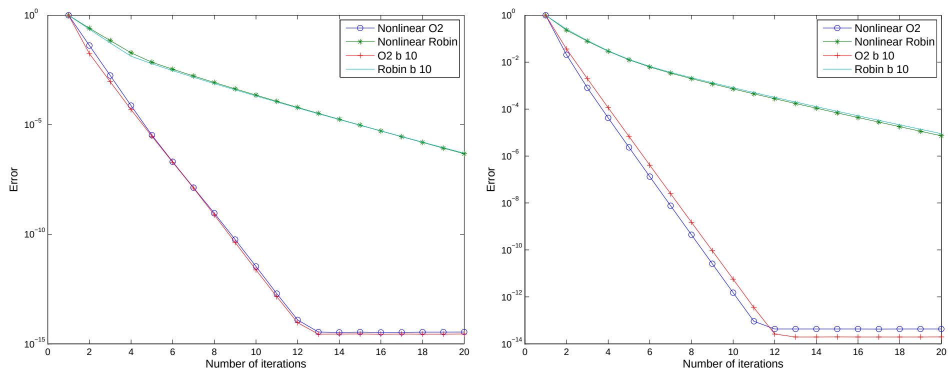

FIGURE 4. For $f(u) = 10(e^u - 1)$, error history in $L^\infty(0, T; L^2(\Omega))$, for $h = 0.0625$ and $h = 0.03125$. Comparison with the optimal parameters for $b = 10$.

5.1. **A simple model in geological CO_2 storage modeling.** We present here a very simple model of a reactive system which can appear in the framework of geological CO_2 storage modeling. We consider a reactive chemical system with two types of materials, evolving according to the equation

$$u_t - \nu \Delta u + f(x, y, u) = 0.$$

The nonlinear function f depends on the spatial variables, describing a heterogeneous distribution of the materials in the spatial domain. Both materials are evolving through equilibrium values u_1^{eq} and u_2^{eq}. The reaction is described here by the function

$$f(x, y, u) = k_1 S_1(x, y)(u - u_1^{eq})^3 + k_2 S_2(x, y)(u - u_2^{eq})^3.$$

The positive constants k_1 and k_2 represent the reaction speeds of material 1 and 2, and the surface functions S_i describe the spatial distribution of the material $i,\ i = 1, 2$. The convergence and well-posedness results of the previous sections can be easily extended to the case of a function f also depending on (x, y).

In the test that we illustrate in Figure 5 below, we considered $k_1 = 5,\ u_1^{eq} = 1,\ k_2 = 3,\ u_2^{eq} = 0,\ S_1(x, y) = \sin(\frac{3\pi}{2}x + \frac{\pi}{2})\sin(\frac{3\pi}{2}y + \frac{\pi}{2})\chi_W$, where W is a zone corresponding to a part of a circle in the spatial domain, and $S_2(x, y) = \max\big(\sin(\frac{5\pi}{2}x + \frac{\pi}{3})\sin(\frac{5\pi}{2}y + \frac{\pi}{3}), 0\big)$. The initial and Dirichlet data are both equal to 0.5. We used here nonlinear transmission conditions, obtained by replacing b with $\partial_u f$ in formulas (39) and (40).

In Figure 6 we compare the results obtained with the nonlinear conditions and with the coefficients of the heat equation for different values of the mesh-spacing h.

As a final test, we illustrate the case where different time scales are considered in the subdomains. We consider uniform time grids in each subdomain with $\Delta t_1 = \frac{\Delta t_2}{2}$, $\Delta t_i,\ i = 1, 2$, being the constant time steps in each domain. The time grid for

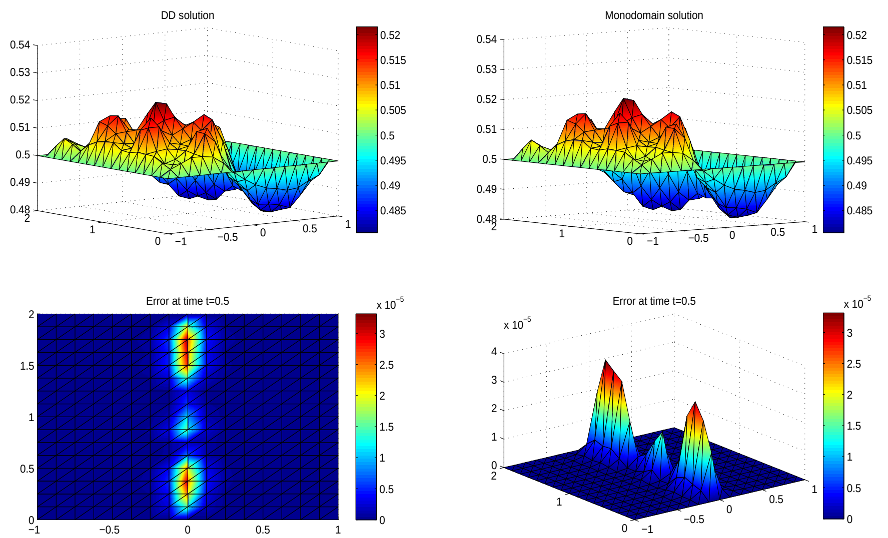

FIGURE 5. Mono-domain solution, domain decomposition solution and error after 10 iterations of the algorithm at time $t = 0.5$

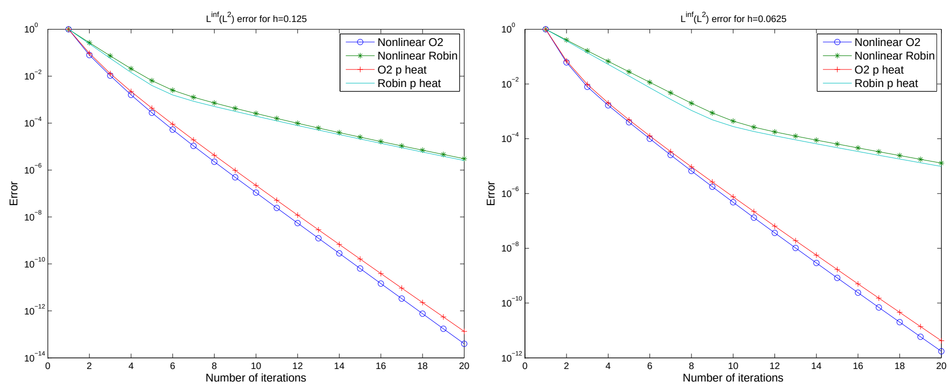

FIGURE 6. Error for $h = 0.125$ and $h = 0.0625$.

the problem in Ω_1 is thus the fine grid and the one for the problem in Ω_2 the coarse grid. At a step k of the iterative domain decomposition algorithm, after solving the initial and boundary value problems in each domain, new boundary values have to be constructed and transmitted to the other domain, for step $k+1$ (cf. [10] for further details). To do so, we perform a first order polynomial interpolation to project the boundary condition vectors between the different time grids. Figure 7 illustrates the behavior of the L^2 error in space between the domain decomposition solution and the mono-domain solution, at final time $t = 1$, as a function of the time steps Δt_i, which are successively divided by a factor of 2. Here h is kept constant and small when compared with the smallest time step. The error is computed as follows : we construct two mono-domain solutions, corresponding to the solutions in the different time grids, and we compute the L^2 error between the domain decomposition solution obtained in each domain Ω_i and the restriction to Ω_i of the mono-domain solution corresponding to the time grid for the problem in $\Omega_i,\ i = 1, 2$. As we can observe in Figure 7, the error decreases linearly with the time step, which was expected since the discretization scheme that we considered in each subdomain is of order 1 in time. Linear Robin transmission conditions were used here and we did 10 iterations of the domain decomposition algorithm. We point out that the optimized transmission conditions that we used previously were obtained by considering the same time and space steps in the whole domain. For the moment, as far as we know, no optimization theory has been developed when different discretizations are used in the different sub-domains.

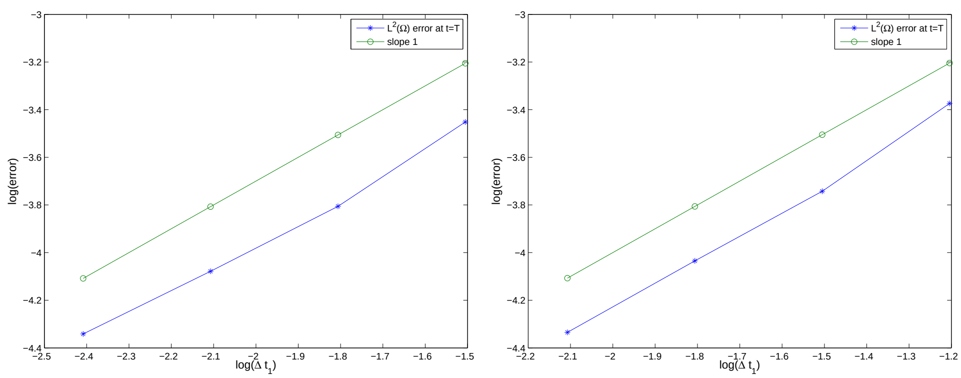

FIGURE 7. L^2 error between mono-domain and domain decomposition solution, at time $t = 1$, as a function of the time step, taken in logarithmic scale, in subdomain Ω_1 (on the left) and Ω_2 (on the right). In x-coordinate $\log_{10}(\Delta t)$ and in y-coordinate $\log_{10}$ of the error.

6. **Conclusion.** We have introduced here new nonoverlapping domain decomposition algorithms for the semilinear heat equation. They extend to nonlinear problems the Schwarz waveform relaxation algorithm, using Robin or Ventcell transmission conditions. Original proofs of well-posedness and convergence have been given for linear transmission. We also proposed nonlinear transmission, which prove numerically to be very efficient. Extensions to reactive transport and Burgers equation are in progress.

Acknowledgments. The authors are grateful to Anthony Michel for providing the reactive transport model of the last section.

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Received xxxx 20xx; revised xxxx 20xx.

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