

Optimized Schwarz waveform relaxation for porous media applications

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1 Introduction

Far field simulations of underground nuclear waste disposal involve a number of challenges for numerical simulations: widely differing lengths and time-scales, highly variable coefficients and stringent accuracy requirements. In the site under consideration by the French Agency for Nuclear Waste Management (ANDRA), the repository would be located in a highly impermeable geological layer, whereas the layers just above and below have very different physical properties (see Alain Bourgeat and Talandier [2004]). It is then natural to use different time steps in the various layers, so as to match the time step with the physics. To do this, we propose to adapt a global in time domain decomposition method, based on Schwarz waveform relaxation algorithms, to problems in heterogeneous media. This method has been introduced and analyzed for linear advection-reaction-diffusion problems with continuous coefficients (Martin [2005], Bennequin et al. [2009]) and extended to discontinuous coefficients (Gander et al. [2007], Halpern et al. [2010]), with asymptotically optimized Robin transmission conditions in Gander et al. [2007]. The method is extended to higher dimension in Halpern et al. [2010] with convergence results and error estimates for rectangular or strip subdomains.

This method is extended to problems with discontinuous porosity in Halpern et al. [Lisbon, Portugal, 14-17 June 2010]. A new approach is proposed to determine optimized transmission conditions for domains with highly variable lengths. In this paper we analyse this approach in 1d.

Our model problem for the radionuclide transport is the one dimensional advection-diffusion-reaction equation

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$$\begin{aligned} \varphi \partial_t u + a \partial_x u - \partial_x(\nu \partial_x u) + bu &= f, & \text{on } \mathbb{R} \times (0, T), \\ u(0, x) &= u_0(x), & x \in \mathbb{R}. \end{aligned} \quad (1)$$

We focus on a model problem to show the effect of subdomains with widely differing sizes. We consider a decomposition in $\Omega_1 = (-\infty, 0)$, $\Omega_2 = (0, L)$, $\Omega_3 = (L, \infty)$ with $L \ll 1$. The reaction coefficient b is taken constant and the coefficients a , ν , and φ are assumed constant on each Ω_i , but may be discontinuous at $x = 0$ and $x = L$,

$$\varphi = \varphi_i, \quad a = a_i, \quad \nu = \nu_i, \quad x \in \Omega_i.$$

We introduce the notations

$$\begin{aligned} \mathcal{L}_i v &:= \varphi_i \partial_t v + a_i \partial_x v - \partial_x(\nu_i \partial_x v) + bv, & \text{on } \Omega_i \times (0, T), \\ \boldsymbol{\varphi} &:= (\varphi_1, \varphi_2, \varphi_3), \quad \mathbf{a} := (a_1, a_2, a_3), \quad \boldsymbol{\nu} := (\nu_1, \nu_2, \nu_3). \end{aligned}$$

Problem (1) is equivalent to solving problems in subdomains Ω_i

$$\begin{aligned} \mathcal{L}_i u_i &= f, & \text{on } \Omega_i \times (0, T), \\ u_i(0, x) &= u_0(x), & x \in \Omega_i. \end{aligned}$$

with coupling conditions on the interface $\Gamma_{i,j}$ between two neighboring subdomains Ω_i and Ω_j given by

$$u_i = u_j, \quad (\nu_i \partial_x - a_i) u_i = (\nu_j \partial_x - a_j) u_j \text{ on } \Gamma_{i,j} \times (0, T). \quad (2)$$

2 Domain decomposition algorithm

A simple algorithm based on relaxation of the coupling conditions (2) does not converge in general (see Quarteroni and Valli [1997]). Following previous works (Gander et al. [2007], Bennequin et al. [2009], Halpern et al. [2010]), we introduce the Schwarz waveform relaxation algorithm

$$\begin{aligned} \mathcal{L}_i u_i^k &= f, & \text{on } \Omega_i \times (0, T), \\ u_i^k(0, x) &= u_0(x), & x \in \Omega_i, \\ (\nu_i \partial_x - a_i) u_i^k + \mathcal{S}_{i,j} u_i^k &= (\nu_j \partial_x - a_j) u_j^{k-1} + \mathcal{S}_{i,j} u_j^{k-1} & \text{on } \Gamma_{i,j} \times (0, T), \end{aligned} \quad (3)$$

where $\mathcal{S}_{i,j}$ are linear operators in time and space, defined by

$$\mathcal{S}_{i,j} \psi = \bar{p}_{i,j} \psi + \bar{q}_{i,j} \partial_t \psi,$$

The case $\bar{q}_{i,j} = 0$ corresponds to Robin transmission conditions, while $\bar{q}_{i,j} \neq 0$ corresponds to first order transmission conditions. The well-posedness and convergence have been analyzed for constant porosity in Gander et al. [2007] and higher dimension and general decomposition in Halpern et al. [2010]. The transmission conditions in (3) imply the coupling conditions (2) at con-

vergence, and lead at the same time to an efficient algorithm, for suitable parameters $\bar{p}_{i,j}$ and $\bar{q}_{i,j}$ obtained from an optimization of the convergence factor.

Similarly, $S_{i,j}$ are approximations of the best operators related to transparent boundary operators. They can be found using Fourier analysis in the two half-spaces case. This analysis has been done for discontinuous coefficients (Gander et al. [2007]), and in higher dimension and continuous coefficients (Bennequin et al. [2009]). The min-max problem has been analysed in one dimension in Gander et al. [2007] with asymptotical Robin parameters.

In the field of nuclear waste computations, domains of meter scale are embedded in domains of kilometer scale. The previous optimization of the convergence factor does not take into account the high variability of the domains lengths. Following Halpern et al. [Lisbon, Portugal, 14-17 June 2010], we determine optimized transmission conditions through the minimization of a convergence factor that takes into account this variability.

2.1 Optimal transmission conditions

In order to determine the optimal transmission operators $S_{i,j}$, we compute the convergence factor of the algorithm. Since the problem is linear, we consider the algorithm (3) on the error (i.e. with $f = 0$ and $u_0 = 0$). In order to use a Fourier transform in time, we assume that all functions are extended by 0 for $t < 0$.

Let $e_i^k = u_i^k - u$ be the error in Ω_i at iteration k . The operators $S_{i,j}$ are related to their symbols $\sigma_{i,j}(\omega)$ by

$$\mathcal{S}_{i,j}u(t) = \frac{1}{2\pi} \int \sigma_{i,j}(\omega) \hat{u}(\omega) e^{i\omega t} d\omega.$$

The Fourier transforms \hat{e}_i^k in time of e_i^k are solutions of the ordinary differential equation in the x variable

$$-\nu_i \partial_{xx}^2 \hat{e} + a_i \partial_x \hat{e} + (i\varphi_i \omega + b) \hat{e} = 0.$$

The characteristic roots are

$$r^\pm(a_i, \nu_i, \varphi_i, \omega) = \frac{a_i \pm \sqrt{d_i}}{2\nu_i}, \quad d_i = a_i^2 + 4\nu_i(i\varphi_i \omega + b). \quad (4)$$

Since $\Re r^+ > 0$, $\Re r^- < 0$, and since we look for solutions which do not increase exponentially in x , we obtain

$$\begin{aligned} \hat{e}_1^k(x, \omega) &= \alpha_1^k(\omega) e^{r^+(a_1, \nu_1, \varphi_1, \omega)x}, & \hat{e}_3^k(x, \omega) &= \alpha_3^k(\omega) e^{r^-(a_3, \nu_3, \varphi_3, \omega)x}, \\ \hat{e}_2^k(x, \omega) &= \alpha_2^k(\omega) e^{r^+(a_2, \nu_2, \varphi_2, \omega)x} + \beta_2^k(\omega) e^{r^-(a_2, \nu_2, \varphi_2, \omega)x}. \end{aligned} \quad (5)$$

We set $\xi^k = (\alpha_1^k, \alpha_2^k, \beta_2^k, \alpha_3^k)^t$, and $r_i^\pm = r^\pm(a_i, \nu_i, \varphi_i, \omega)$. We define the variables $s_i = s_i(\omega, L)$, $1 \leq i \leq 8$, by

$$\begin{aligned} s_1 &= \frac{a_2 - \nu_2 r_2^+ - \sigma_{1,2}}{a_1 - \nu_1 r_1^+ - \sigma_{1,2}}, \quad s_2 = \frac{a_2 - \nu_2 r_2^- - \sigma_{1,2}}{a_1 - \nu_1 r_1^+ - \sigma_{1,2}}, \quad s_3 = \frac{a_2 - \nu_2 r_2^- - \sigma_{2,3}}{a_2 - \nu_2 r_2^+ - \sigma_{2,3}} \cdot e^{(r_2^- - r_2^+)L} \\ s_5 &= \frac{a_2 - \nu_2 r_2^+ + \sigma_{2,1}}{a_2 - \nu_2 r_2^- + \sigma_{2,1}}, \quad s_7 = \frac{a_2 - \nu_2 r_2^+ + \sigma_{3,2}}{a_3 - \nu_3 r_3^- + \sigma_{3,2}} e^{(r_2^+ - r_3^-)L}, \quad s_8 = \frac{a_2 - \nu_2 r_2^- + \sigma_{3,2}}{a_3 - \nu_3 r_3^- + \sigma_{3,2}} e^{(r_2^- - r_3^-)L}, \\ s_4 &= \frac{a_1 - \nu_1 r_1^+ + \sigma_{2,1}}{a_2 - \nu_2 r_2^- + \sigma_{2,1}} \cdot \frac{1}{D}, \quad s_6 = \frac{a_3 - \nu_3 r_3^- - \sigma_{2,3}}{a_2 - \nu_2 r_2^+ - \sigma_{2,3}} \cdot \frac{e^{(r_3^- - r_2^+)L}}{D}, \quad \text{with } D = s_3 s_5 - 1. \end{aligned}$$

We insert (5) into the transmission conditions in (3), and obtain for $k \geq 2$,

$$\xi^k = M \xi^{k-1},$$

where the matrix $M = M(\omega, L)$ is defined by

$$M = \begin{pmatrix} 0 & s_1 & s_2 & 0 \\ s_3 s_4 & 0 & 0 & -s_6 \\ -s_4 & 0 & 0 & s_5 s_6 \\ 0 & s_7 & s_8 & 0 \end{pmatrix}.$$

The convergence factor $\rho(\omega, L)$ for each $\omega \in \mathbb{R}$ is the spectral radius of M .

Remark 1. The choice for the symbols $\sigma_{i,j}$

$$\begin{aligned} \sigma_{1,2} &= a_2 - \nu_2 r_2^-, & \sigma_{2,1} &= -a_1 + \nu_1 r_1^+, \\ \sigma_{2,3} &= a_3 - \nu_3 r_3^-, & \sigma_{3,2} &= -a_2 + \nu_2 r_2^+, \end{aligned} \quad (6)$$

leads to $M^2 = 0$ and thus to optimal convergence in three iterations.

Lemma 1. *The convergence factor is given by*

$$\rho(\omega, L) = \sqrt{\max(|\lambda^-|, |\lambda^+|)},$$

where $\lambda^\pm = \lambda^\pm(\omega, L)$ is defined by

$$\lambda^\pm = \frac{\alpha + \beta \pm \sqrt{(\alpha - \beta)^2 + 4\gamma\zeta}}{2},$$

with

$$\alpha = s_1 s_3 s_4 - s_2 s_4, \quad \beta = -s_6 s_7 + s_5 s_6 s_8, \quad \gamma = s_3 s_4 s_7 - s_4 s_8, \quad \zeta = -s_1 s_6 + s_2 s_5 s_6.$$

The corresponding operators to (6) are non-local in time. In the next subsection, we therefore approximate the optimal operators by local ones.

2.2 Local transmission conditions

We approximate the optimal choice $\sigma_{i,j}$ in (6) by polynomials in ω :

$$\begin{aligned}\sigma_{1,2}^{\text{app}} &= \frac{p_{1,2} + a_2}{2} + \frac{q_{1,2}}{2}i\omega, & \sigma_{2,1}^{\text{app}} &= \frac{p_{2,1} - a_1}{2} + \frac{q_{2,1}}{2}i\omega, \\ \sigma_{2,3}^{\text{app}} &= \frac{p_{2,3} + a_3}{2} + \frac{q_{2,3}}{2}i\omega, & \sigma_{3,2}^{\text{app}} &= \frac{p_{3,2} - a_2}{2} + \frac{q_{3,2}}{2}i\omega.\end{aligned}$$

In order to simplify the min-max problem, we will consider the following cases for the choice of $p_{i,j}$ and $q_{i,j}$:

1. (Robin) $p_{i,j} = p$, $q_{i,j} = 0$,
2. (Zeroth order) $p_{1,2} = p_{3,2} = p_1$, $p_{2,1} = p_{2,3} = p_2$, $q_{i,j} = 0$,
3. (First order) $p_{i,j} = p$, $q_{i,j} = q$,
4. (First order scaled) $p_{i,j} = p$, $q_{1,2} = \varphi_2 q$, $q_{2,1} = \varphi_1 q$, $q_{2,3} = \varphi_3 q$, $q_{3,2} = \varphi_2 q$.

Then, the parameters are chosen in order to minimize the convergence factor, i.e. we solve, for $\mathbf{p} = p$ in case 1, $\mathbf{p} = (p_1, p_2)$ in case 2, and $\mathbf{p} = (p, q)$ in cases 3 and 4, the min-max problem

$$\delta_n(L) = \min_{\mathbf{p}} \left(\max_{\omega_0 \leq \omega \leq \omega_{\max}} \rho(\omega, \mathbf{p}, \boldsymbol{\varphi}, \mathbf{a}, \boldsymbol{\nu}, b, L) \right), \quad (7)$$

where ρ is the spectral radius of M , in which we have replaced $\sigma_{i,j}$ by $\sigma_{i,j}^{\text{app}}$, and n is the order of the approximation. In numerical computations, the frequencies can be restricted to $\omega_{\max} = \frac{\pi}{\Delta t}$, where Δt is the time step, and $\omega_0 = \frac{\pi}{T}$.

Theorem 1. *If $a_i = a$, $\varphi_i = \varphi$ and $\nu_i = \nu$ $1 \leq i \leq 3$, then $d_i = d$ in (4) and the convergence factor reduces to*

$$\rho(\omega, L) = \sqrt{\left| \frac{\sigma - \sqrt{d}}{\sigma + \sqrt{d}} \right| \max \left(\left| \frac{\sigma - \mu}{\sigma + \mu} \right|, \left| \frac{\sigma - \eta}{\sigma + \eta} \right| \right)} \quad (8)$$

with

$$\mu = \sqrt{d} \left(\frac{1 + e^{-\frac{\sqrt{d}}{2\nu}L}}{1 - e^{-\frac{\sqrt{d}}{2\nu}L}} \right), \quad \eta = \frac{\sqrt{d}}{\mu}. \quad (9)$$

Theorem 2. *Let $L > 0$ given. Let $\delta_0(L)$ (resp. $\delta_1(L)$) be the solution of (7) for the Robin case (resp. the first order case). If $a_i = a$, $\varphi_i = \varphi$ and $\nu_i = \nu$, $1 \leq i \leq 3$, for $n = 0$ and $n = 1$, we have $|\delta_n(L)| < 1$.*

3 Numerical results

We use the DG-OSWR method in Halpern et al. [2010] based on a discontinuous Galerkin method in time, with \mathbf{P}_1 finite elements in space in each subdomain. We present an example inspired from nuclear waste simulations, with discontinuous coefficients, and different time and space steps in the subdomains $\Omega_2 = (0.4954, 0.5047)$ (repository), $\Omega_1 = (0, 0.4954)$ and $\Omega_3 = (0.5047, 1)$ (host rock). The parameters for the three subdomains are shown in Table 1. The final time is $T = 0.04$.

	φ	ν	a	b	Δx	Δt
$\Omega_1 \cup \Omega_3$	0.06	0.06	1	0	10^{-2}	$T(5 \cdot 10^{-3})$
Ω_2	0.1	1	1	0	10^{-3}	$T(2 \cdot 10^{-3})$

Table 1. Physical and numerical parameters.

Let \mathbf{p}_3^* (resp. \mathbf{p}_2^*) be the parameters derived from a numerical minimization of the three domains convergence factor in (7) (resp. from the two half-spaces convergence factor in Gander et al. [2007]). Figure 1 shows $\rho(\omega, \mathbf{p}_3^*, L)$ (solid line) and $\rho(\omega, \mathbf{p}_2^*, L)$ (dashed line) versus w for $\Delta t = T(5 \cdot 10^{-3})$. We observe

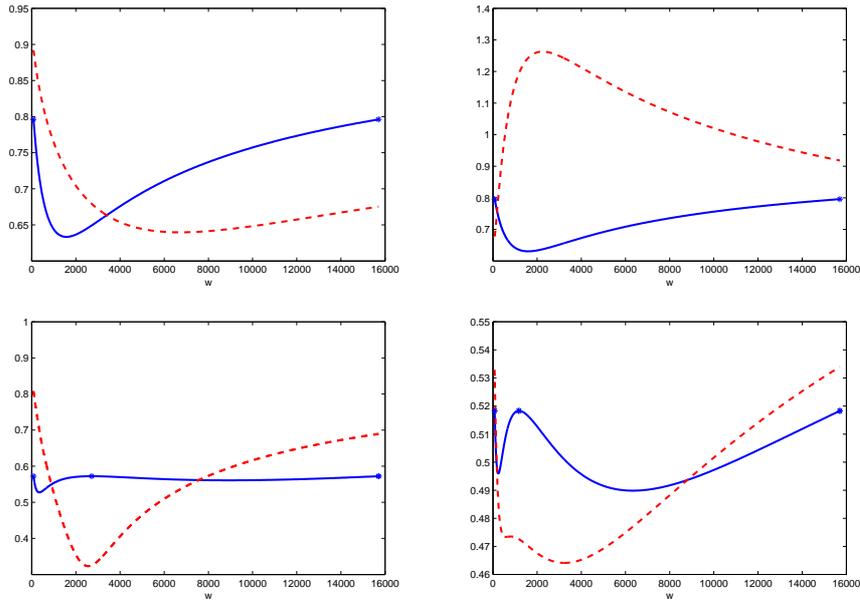


Fig. 1 Convergence factor $\rho(w, \mathbf{p}_3^*)$ (solid line) and $\rho(w, \mathbf{p}_2^*)$ (dashed line) versus w : Top left: Robin, top right: zeroth order, left bottom: first order, right bottom: first order scaled.

that the solution of (7) is characterized by an equioscillation property (at

the star marks), as in the two half-spaces case (see Bennequin et al. [2009]). Moreover, for first order transmission conditions, we see that a scaling with the porosity is important only when the parameters are computed from the two half-spaces analysis.

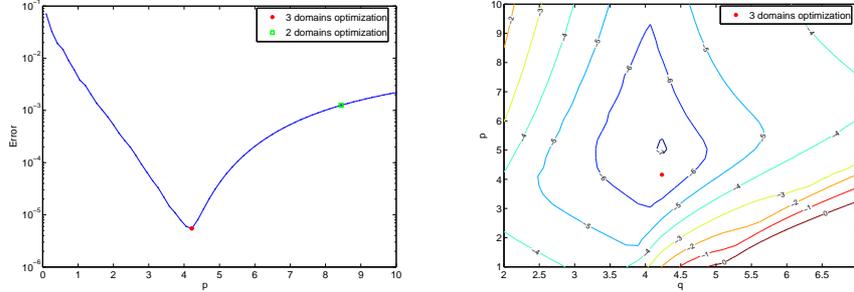


Fig. 2 Error after 20 iterations: Left: for various values of the Robin parameter p (the lower left star marks p_3^* whereas the upper right square shows p_2^*), Right: the level curves for various values of the zeroth order parameters p_1, p_2 (the star marks the parameter p_3^*).

On Figure 2 we show the error after 20 iterations when running the algorithm on the discretized problem, with $u_o = f = 0$ and random initial guess on the interfaces, for various values of the Robin parameter p (left) and the zeroth order parameters p_1, p_2 (right) (in that case, the values obtain with the two half-spaces analysis is not in the range values of the figure).

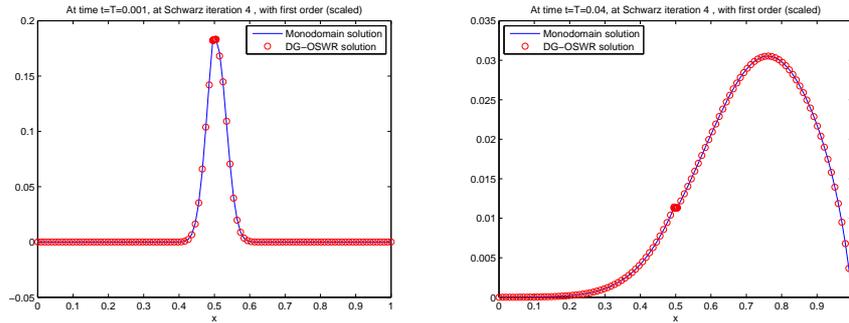


Fig. 3 Evolution of the monodomain solution (solid line) and the OSWR solution at iteration 4 (circle line): at $t = 0.001$ (left), $t = T = 0.04$ (right)

On Figure 3, the solution, with first order (scaled) conditions, at iteration 4 is shown for an initial condition equal to 1 in Ω_2 and 0 elsewhere.

Figure 4 shows on the left $R(\Delta t) = 1 - \max_{\pi/T \leq \omega \leq \pi/\Delta t} \rho(w, L, \mathbf{p}_3^*)$ versus Δt , i.e. the convergence factor behave like $1 - O(\Delta t)^{1/16}$, with first order (scaled) optimized transmission conditions. On the right, we run the OSWR algorithm until the error becomes smaller than 10^{-11} , and count the number of iterations. We start with $\Delta t = T/100$ in each subdomain, and repeat this experiment dividing Δx and Δt by 2 several times. We observe that the

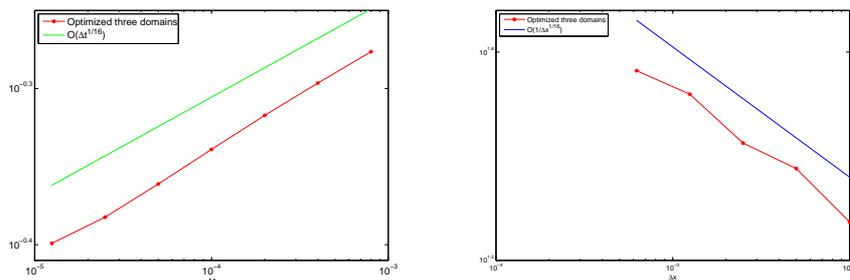


Fig. 4 Asymptotic behavior as the mesh is refined: on the left $R(\Delta t)$ and on the right where $\Delta t = O(\Delta x)$, the rate for the optimized Schwarz waveform relaxation algorithm with optimized first order (scaled) transmission conditions.

asymptotic result on the left predicts very well the numerical behavior of the algorithm given on the right.

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