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A Schwarz Waveform Relaxation Method for Advection–Diffusion–Reaction Problems with Discontinuous Coefficients and non-Matching Grids

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Summary. We present a non-overlapping Schwarz waveform relaxation method for solving advection-reaction-diffusion problems in heterogeneous media. The domain decomposition method is global in time, which permits the use of different time steps in different subdomains. We determine optimal non-local, and optimized Robin transmission conditions. We also present a space-time finite volume scheme especially designed to handle such transmission conditions. We show the performance of the method on an example inspired from nuclear waste disposal simulations.

1 Motivation and Problem Setting

What to do with nuclear waste is a question being addressed by several organizations worldwide. Long term storage within a deep geological formation is one of the possible strategies, and Andra, the French Agency for Nuclear Waste Management, is currently carrying out feasibility studies for building such a repository. Given the time span involved (several hundreds of thousands, even millions, of years), physical experiments are at best difficult, and one must resort to numerical simulations to evaluate the safety of a proposed design.

Deep disposal of nuclear waste raises 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 Andra, the repository would be located in a highly impermeable geological layer, whereas the layers just above and below have very different physical properties. In the clay layer, the radionuclides move essentially because of diffusion, whereas in the dogger layer that is above the main phenomenon is

advection (see [BKST04] and the other publications in the same issue for a detailed discussion of numerical methods that can be applied to a simplified, though relevant, situation).

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 proposed by Gander and Halpern in [BGH04] (see also [GHN03], and [Mar04] for a different application) to the case of a model with discontinuous coefficients. The main advantage of the method is that it allows us to take different time steps in the subdomains, while only synchronizing at the end of the time simulation.

Our model problem is the one dimensional advection–diffusion–reaction equation

$$\begin{aligned} \mathcal{L}u &:= \frac{\partial u}{\partial t} - \frac{\partial}{\partial x} \left(D \frac{\partial u}{\partial x} - au \right) + bu = f, & \text{on } \mathbf{R} \times [0, T], \\ u(x, 0) &= u_0(x), & x \in \mathbf{R}, \end{aligned} \quad (1)$$

where the reaction coefficient b is taken constant and the coefficients a and D are assumed constant on each half line \mathbf{R}^+ and \mathbf{R}^- , but may be discontinuous at 0,

$$a = \begin{cases} a^+ & x \in \mathbf{R}^+, \\ a^- & x \in \mathbf{R}^-, \end{cases} \quad D = \begin{cases} D^+ & x \in \mathbf{R}^+, \\ D^- & x \in \mathbf{R}^-. \end{cases} \quad (2)$$

If $u_0 \in L^2(\mathbf{R})$ and $f \in L^2(0, T; L^2(\mathbf{R}))$, then problem (1) has a unique weak solution $u \in L^\infty(0, T; L^2(\mathbf{R})) \cap L^2(]0, T[; H^1(\mathbf{R}))$, see [LM72]. In the sequel, it will be convenient to use the notation

$$\begin{aligned} \mathcal{L}^\pm v &:= \frac{\partial v}{\partial t} - \frac{\partial}{\partial x} \left(D^\pm \frac{\partial v}{\partial x} - a^\pm v \right) + bv, & x \in \mathbf{R}^\pm, t > 0, \\ \mathcal{B}^\pm v &:= \mp D^\pm \frac{\partial v}{\partial x} \pm a^\pm v, & x = 0, t > 0. \end{aligned} \quad (3)$$

One can show that (1), (2) is equivalent to the decomposed problem

$$\begin{aligned} \mathcal{L}^- u^- &= f, & \text{on } \mathbf{R}^- \times [0, T], & \quad \mathcal{L}^+ u^+ = f, & \text{on } \mathbf{R}^+ \times [0, T], \\ u^-(x, 0) &= u_0(x), & x \in \mathbf{R}^-, & \quad u^+(x, 0) = u_0(x), & x \in \mathbf{R}^+, \end{aligned} \quad (4)$$

together with the *coupling conditions*

$$u^+(0, t) = u^-(0, t), \quad \mathcal{B}^+ u^+(0, t) = -\mathcal{B}^- u^-(0, t), \quad t \in [0, T]. \quad (5)$$

2 Domain Decomposition Algorithm

A simple algorithm based on relaxation of the coupling conditions (5) does not converge in general, not even in the simpler cases, see for example [QV99]. Instead of introducing a relaxation parameter, as in the classical Dirichlet–Neumann method, we introduce *transmission conditions* which imply the coupling conditions in (5) at convergence, and lead at the same time to an effective

iterative method. We introduce two operators Λ^+ and Λ^- acting on functions defined on $[0, T]$, such that

$$\forall g \in L^2(\mathbf{R}), \widehat{\Lambda^\pm g}(\omega) = \lambda^\pm(\omega)\widehat{g}(\omega), \forall \omega \in \mathbf{R},$$

where \widehat{g} is the Fourier transform of the function g , and λ^\pm is the *symbol* of Λ^\pm . For $k = 0, 1, 2, \dots$, we consider the Schwarz waveform relaxation algorithm

$$\begin{aligned} \mathcal{L}^+ u_{k+1}^+ &= f, & \text{on } \mathbf{R}^+ \times [0, T], \\ u_{k+1}^+(x, 0) &= u_0(x), & x \in \mathbf{R}^+, \\ (\mathcal{B}^+ + \Lambda^+) u_{k+1}^+(0, t) &= (-\mathcal{B}^- + \Lambda^+) u_k^-(0, t), & t \in [0, T], \\ \mathcal{L}^- u_{k+1}^- &= f, & \text{on } \mathbf{R}^- \times [0, T], \\ u_{k+1}^-(x, 0) &= u_0(x), & x \in \mathbf{R}^-, \\ (\mathcal{B}^- + \Lambda^-) u_{k+1}^-(0, t) &= (-\mathcal{B}^+ + \Lambda^-) u_k^+(0, t), & t \in [0, T]. \end{aligned} \quad (6)$$

If this algorithm converges, then, provided $\Lambda^+ - \Lambda^-$ has a null kernel, the limit is a solution of the coupled problem (4), (5), and hence of the original problem (1).

2.1 Optimal Transmission Conditions

In order to choose the transmission operators Λ^+ and Λ^- , we first determine the convergence factor of the algorithm. Since the problem is linear, the error equations coincide with the homogeneous equations, that is we may take $f = 0$ and $u_0 = 0$ in algorithm (6) above. In order to use Fourier transforms in time, we assume that all functions are extended by 0 for $t < 0$. Denoting the errors in \mathbf{R}^\pm by e_k^\pm , we see that the Fourier transforms of e_k^+ and e_k^- are given by

$$\begin{aligned} \widehat{e}_k^-(x, \omega) &= \beta_k(\omega) e^{r^+(a^-, D^-, \omega)x}, & (x, \omega) \in \mathbf{R}^- \times \mathbf{R}, \\ \widehat{e}_k^+(x, \omega) &= \alpha_k(\omega) e^{r^-(a^+, D^+, \omega)x}, & (x, \omega) \in \mathbf{R}^+ \times \mathbf{R}, \end{aligned} \quad (7)$$

where α_k and β_k are determined by the transmission conditions, and $r^+(a, D, \omega)$ and $r^-(a, D, \omega)$ are the roots with positive and negative real parts of the characteristic equation

$$Dr^2 - ar - (b + i\omega) = 0. \quad (8)$$

If we substitute (7) into the transmission conditions of algorithm (6), we obtain over a double step of the algorithm

$$\alpha_{k+1}(\omega) = \rho(\omega)\alpha_{k-1}(\omega), \quad \beta_{k+1}(\omega) = \rho(\omega)\beta_{k-1}(\omega) \quad (9)$$

with the convergence factor $\rho(\omega)$ for each $\omega \in \mathbf{R}$ given by

$$\rho(\omega) = \frac{a^- - D^- r^+(a^-, D^-, \omega) + \lambda^+(\omega)}{a^- - D^- r^-(a^+, D^+, \omega) + \lambda^+(\omega)} \cdot \frac{a^+ - D^+ r^-(a^+, D^+, \omega) - \lambda^-(\omega)}{a^- - D^- r^+(a^-, D^-, \omega) - \lambda^-(\omega)}. \quad (10)$$

Remark 1. The previous equation shows that there is a choice for λ^\pm that leads to convergence in two iterations. However, the corresponding operators are non-local in time (because of the square-root in $r^\pm(a, D, \omega)$). In the next Subsection, we therefore approximate the optimal operators by local ones.

2.2 Local Transmission Conditions

We approximate the square roots in the roots of (8) by parameters p^\pm which leads to

$$\lambda_{\text{app}}^+(\omega) = \frac{p^- - a^-}{2} \quad \text{and} \quad \lambda_{\text{app}}^-(\omega) = \frac{p^+ + a^+}{2}, \quad \forall \omega \in \mathbf{R}, \quad (11)$$

and hence leads to Robin transmission conditions in algorithm (6).

We call the left *subdomain problem* the system formed by the first two equations of (4), together with the boundary condition

$$(\mathcal{B}^- + \lambda_{\text{app}}^-)u^-(0, t) = g^-, \quad \text{for } t > 0,$$

and similarly for the right subdomain problem. As the coefficients are constants in each subdomain, we can prove the following result exactly as in [BGH04] (see Theorem 5.3, and also [LM72] for the definition of the anisotropic Sobolev space $H^{2,1}(\mathbf{R}^- \times (0, T))$).

Theorem 1 (Well Posedness of Subdomain Problems). *Let $u_0 \in H^1(\mathbf{R})$, $f \in L^2(0, T; \mathbf{R})$, and $g^\pm \in H^{1/4}(0, T)$. Then, for any real numbers λ_{app}^\pm , the subdomain problems have unique solutions $u^\pm \in H^{2,1}(\mathbf{R}^- \times (0, T))$.*

Therefore the subdomain solutions are smooth enough to apply the transmission operators and this proves by induction that algorithm (6) with the Robin transmission conditions (11) is well defined (see also Theorem 5.4 in [BGH04]).

Theorem 2 (Well Posedness of the Algorithm). *Let $f \in L^2(0, T; \mathbf{R})$, $u_0 \in H^1(\mathbf{R})$, and the initial guesses $u_0^\pm \in H^{2,1}(\mathbf{R}^- \times (0, T)) \times H^{2,1}(\mathbf{R}^+ \times (0, T))$. Then, for any real numbers p^\pm , algorithm (6) with Robin transmission conditions (11) is well defined in $H^{2,1}(\mathbf{R}^- \times (0, T)) \times H^{2,1}(\mathbf{R}^+ \times (0, T))$.*

Convergence of the algorithm follows from energy estimates similar to the ones in [BGH04], where however the additional difficulty due to the discontinuities leads to additional constraints on the parameters.

Theorem 3 (Convergence of the Algorithm). *If the three following constraints are satisfied: $\lambda_{\text{app}}^- + \lambda_{\text{app}}^+ > 0$, $\lambda_{\text{app}}^- - \lambda_{\text{app}}^+ + \frac{a^+}{2} \geq 0$, $\lambda_{\text{app}}^- - \lambda_{\text{app}}^+ + \frac{a^-}{2} \leq 0$, then algorithm (6), with Robin transmission conditions (11), is convergent.*

Note that in the case of constant coefficients, and $p^+ = p^- = p$, the constraints reduce to $p > 0$, which is consistent with results in [BGH04].

How should the parameters p^\pm be chosen? A simple approach is to use a low frequency approximation, obtained by a Taylor expansion of the square roots in the roots of (8), which leads to

$$p^+ = \sqrt{(a^+)^2 + 4D^+b}, \quad p^- = \sqrt{(a^-)^2 + 4D^-b}. \quad (12)$$

Such transmission conditions are however not very effective for high frequencies. A better approach is to minimize the convergence factor, i.e. to solve the min-max problem

$$\min_{p^+, p^-} \left(\max_{0 \leq \omega \leq \omega_{\max}} |\rho(\omega, p^+, p^-, a^+, a^-, D^+, D^-, b)| \right), \quad (13)$$

where ρ is given in (10). As we are working with a numerical scheme, the frequencies cannot be arbitrarily high, but can be restricted to $\omega_{\max} = \pi/\Delta t$.

Theorem 4. *If $p^+ = p^- = p$, then for $a^+, a^- > 0$ the solution of the min-max problem (13) is for Δt small given by*

$$p \approx \frac{\left(2^3 \pi (D^+ D^-) (\sqrt{D^+} + \sqrt{D^-})^2 (a^+ - a^- + \sqrt{(a^+)^2 + 4D^+ b} + \sqrt{(a^-)^2 + 4D^- b})^2 \right)^{\frac{1}{4}}}{\sqrt{D^+} + \sqrt{D^-}} \Delta t^{-\frac{1}{4}}, \quad (14)$$

which leads to the asymptotic bound on the convergence factor

$$|\rho| \leq 1 - \left(\frac{2^5 (\sqrt{D^+} + \sqrt{D^-})^2 (a^+ - a^- + \sqrt{(a^+)^2 + 4D^+ b} + \sqrt{(a^-)^2 + 4D^- b})^2}{D^+ D^- \pi} \right)^{\frac{1}{4}} \Delta t^{\frac{1}{4}}. \quad (15)$$

Theorem 5. *If $D^+ = D^- = D$, then for $a^+, a^- > 0$ the solution of the min-max problem (13) is for Δt small given by*

$$\begin{aligned} p^+ &\approx (2^9 \pi^3 D^3 (a^+ - a^- + \sqrt{(a^+)^2 + 4Db} + \sqrt{(a^-)^2 + 4Db})^2)^{\frac{1}{8}} \Delta t^{-\frac{3}{8}}, \\ p^- &\approx (2^{-5} \pi D (a^+ - a^- + \sqrt{(a^+)^2 + 4Db} + \sqrt{(a^-)^2 + 4Db})^6)^{\frac{1}{8}} \Delta t^{-\frac{1}{8}}, \end{aligned} \quad (16)$$

which leads to the asymptotic bound on the convergence factor

$$|\rho| \leq 1 - \left(\frac{2^{13} (a^+ - a^- + \sqrt{(a^+)^2 + 4Db} + \sqrt{(a^-)^2 + 4Db})^2}{D \pi} \right)^{\frac{1}{8}} \Delta t^{\frac{1}{8}}. \quad (17)$$

The most general case where $p^+ \neq p^-$ and D^\pm are arbitrary is asymptotically the most interesting one, since the discontinuity in D changes the exponent in the asymptotically optimal parameter and hence in the convergence factor. This case is currently under investigation.

3 Finite Volume Discretization of the Algorithm

We discretize the subdomain problem by a space-time finite volume method, implicit in time and upwind for the advective part. We denote the space and time steps by Δx , Δt , the grid points by $x_j = j\Delta x$, $j = 0, \dots, N_x$ (with $N_x \Delta x = L$), and $t^n = n\Delta t$, $n = 0, \dots, N_t$, (with $N_t \Delta t = T$). We also let $u_h = (u_j^n)_{(j,n)}$ be the approximate solution, with $u_j^n \approx u(x_j, t^n)$. We consider u_h as

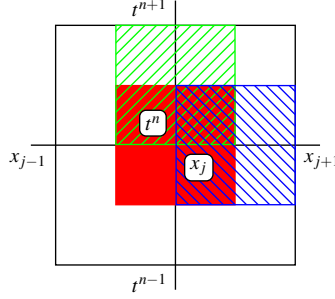


Fig. 1. Finite volume grid. Function is constant on solid rectangle, x -derivative on right-hashed rectangle, t -derivative on left-hashed rectangle.

a constant function on each rectangle $R_j^n = (x_{j-1/2}, x_{j+1/2}) \times (t^{n-1/2}, t^{n+1/2})$ (the fully shaded rectangle in Figure 1). The discrete derivatives are defined by the difference quotient, and are constant on staggered grids, as indicated in Figure 1. Last, we let $u_j^{n+1/2} = \frac{u_j^n + u_j^{n+1}}{2}$.

The discrete scheme for interior points in each subdomain is obtained by integrating the partial differential equation in (6) over the rectangle R_j^n and then using standard finite volume approximations, which leads to

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} - D \frac{u_{j+1}^{n+1/2} - 2u_j^{n+1/2} + u_{j-1}^{n+1/2}}{\Delta x^2} + a \frac{u_j^{n+1/2} - u_{j-1}^{n+1/2}}{\Delta x} + b u_j^{n+1/2} = f_j^{n+1/2}. \quad (18)$$

The scheme can be shown to be unconditionally stable, and first order accurate [GHK05].

The main interest of the finite volume method is that we can handle the transmission conditions in (6) in a natural way. Now we just integrate over half the cell, for example on the right subdomain, and use the transmission condition on the cell boundary on the left, to obtain

$$\frac{\Delta x}{2} \frac{u_0^{n+1} - u_0^n}{\Delta t} - D \frac{u_1^{n+1/2} - u_0^{n+1/2}}{\Delta x} + a u_0^{n+1/2} + \frac{\Delta x}{2} b u_0^{n+1} + \lambda_{\text{app}} u_0^{n+1/2} = g^{n+1/2}, \quad (19)$$

and similarly over the left subdomain. In the same way, we obtain an expression for the operator on the right hand side of the transmission condition. One can show that if the entire domain is homogeneous, then the scheme with the discrete boundary conditions coincides with the interior scheme applied at the interface node [GHK05].

Since the space and time steps will usually be different on the two sides of the interface, we introduce an L^2 projection operator on the boundary (acting on step functions defined in the time domain), as was done in [GHN03].

4 Numerical Experiments

We present an example of the behavior of our algorithm, with discontinuous coefficients, and different time and space steps in the two subdomains. The parameters for the two subdomains are shown in Table 1. Several snapshots of the solution, at 3 different times, and for two different iterations are shown in Figure 2.

	D	a	p	Δx	Δt
Left subdomain \mathbf{R}^-	$4 \cdot 10^{-2}$	4	18.5	10^{-2}	$4 \cdot 10^{-3}$
Right subdomain, \mathbf{R}^+	$12 \cdot 10^{-2}$	2	6.4	$2 \cdot 10^{-2}$	$2 \cdot 10^{-3}$

Table 1. Physical and numerical parameters for an example.

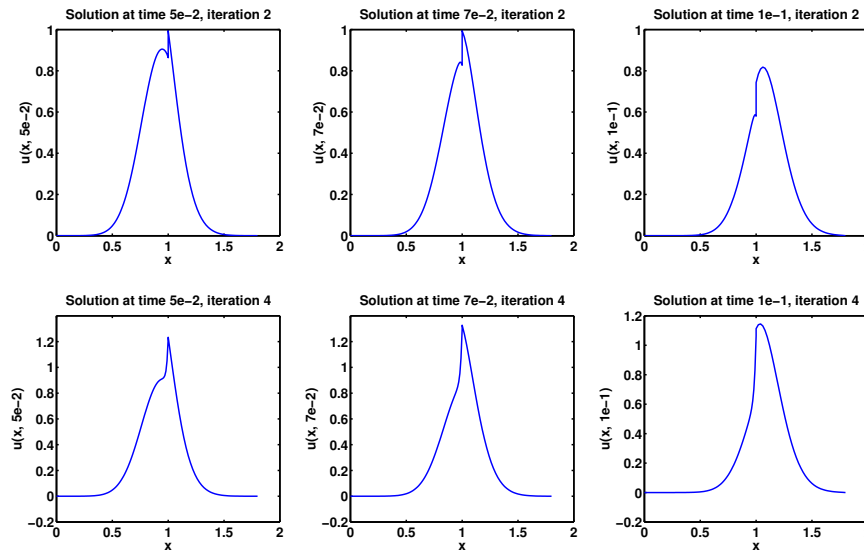


Fig. 2. Evolution of the solution at two different iterations. Top row: iteration 2, bottom row: iteration 4. Left column: $t = 0.05$, middle column $t = 0.07$, right column $t = 0.1$.

Last, to illustrate Theorem 5, we show in Figure 3 the number of iterations needed to reduce the residual by 10^6 when running the algorithm on the discretized problem, for various values of the parameters p^+ and p^- . The parameters corresponding to Theorem 5 and to the values found by minimizing the continuous convergence factor (10) are both shown in the figure (we use the same values as in Table 1 above, except that now $D^+ = D^- = 4 \cdot 10^{-2}$).

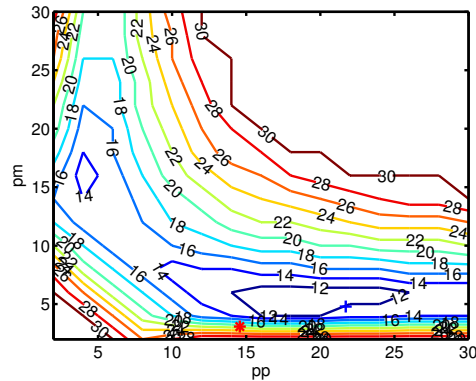


Fig. 3. Level curves for the number of iterations needed to reach convergence for various values of the parameters p^- and p^+ . The lower left star marks the parameters derived from Theorem 5, whereas the upper right cross shows the "optimal" parameters, as found by numerically minimizing the continuous convergence rate.

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