Nonlinear Transmission Conditions for time Domain Decomposition Method

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1 Introduction

We developed parallel time domain decomposition methods to solve systems of linear ordinary differential equations (ODEs) based on the Aitken-Schwarz [7] or primal Schur complement domain decomposition methods [6]. The methods claim the transformation of the initial value problem in time defined on $]0,T]$ into a time boundary values problem. Let $f(t,y(t))$ be a function belonging to $\mathscr{C}^1(\mathbb{R}^+,\mathbb{R}^d)$ and consider the Cauchy problem for the first order ODE:

$$\left\{ \dot{y} = f(t,y(t)),\, t \in]0,T],\; y(0) = y_0 \in \mathbb{R}^d. \right. \tag{1}$$

The time interval $[0,T]$ is split into p time slices $S_i = [T_{i-1}^+, T_i^-]$, with $T_0^+ = 0$ and $T_p^- = T^-$. The difficulty is to match the solutions $y_i(t)$ defined on S_i at the boundaries T_{i-1}^+ and T_i^-. Most of time domain decomposition methods are shooting methods [1] where the jumps $y_i(T_i^-) - y_{i+1}(T_i^+)$ are corrected by a sequential process which is propagated in the forward direction (i.e. the correction on the time slice S_{i-1} is needed to compute the correction on time slice S_i). Our approach consists in breaking the sequentiality of the solution's initial value updating for each time slice. For this, we transform the initial value problem (IVP) into a boundary values problem (BVP) leading to a second order ODE:

$$\ddot{y}(t) = g(t,y(t)) \overset{def}{=} \frac{\partial f}{\partial t}(t,y) + f(t,y(t))\frac{\partial f}{\partial y}(t,y(t)),\, t \in]0,T[, \tag{2a}$$

$$y(0) = y_0, \tag{2b}$$

$$y(T) = \beta. \tag{2c}$$

Nevertheless, the difficulty in solving equation (2) is that β is not given by the original IVP. To overcome the lack of knowledge of β, we proposed to set this value by using an iterative Schwarz domain decomposition method with no overlapping. For sake of simplicity, let us consider only one domain S_1. Given a,b in $\mathbb{R}^+$ with

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$a < b$, we denote $\overline{[a,b]}$ to indicate that the time interval must be traveled in the backward direction. We first symmetrize the time interval S_1 providing $\bar{S}_1 = \overline{[0^+, T^-]}$. A symmetric time integration scheme, like the second order implicit Störmer-Verlet symmetric scheme, is then required to perform a backward time integration onto the symmetrized interval to come back to the initial state. Then classical domain decomposition methods can be applied such the multiplicative Schwarz method with no overlapping time slices with Dirichlet-Neumann (associated to the Laplacian in time) transmission conditions (T.C.) for linear system of ODE (or PDE [8]). As proved in [7] the convergence/divergence of the error at the boundaries of this Schwarz time DDM can be accelerated by the Aitken technique to the right solution when $f(t,y(t))$ is linear.

This paper treats the case where $f(t,y(t))$ is nonlinear. Then the multiplicative Schwarz algorithm generates at the boundary of time slices a nonlinear vectorial sequence. We replaced in [5] the Aitken's acceleration of the convergence by the ε-topological algorithm [3] that has been designed to extrapolate the convergence of such nonlinear sequences. Some enhancement of the convergence have been obtained but the number of Schwarz iterations is still too large to obtain an efficient method. This leads us to think again about the transmission conditions between time slices. When systems of nonlinear ODEs are under consideration, we show in the next section that the Dirichlet-Neumann T.C. (associated to the time Laplacian operator only) at boundary time slices are not the right choice. The Neumann boundary condition has to be replaced by a nonlinear boundary condition preserving an invariant of the solution. These nonlinear T.C. differ from the optimized nonlinear T.C. present in the waveform relaxation of [4]. In section 3, we show the pure linear behavior of the multiplicative Schwarz with a combination of the nonlinear T.C. and the Dirichlet condition by demonstrating that the operator associated to the error does not depend of the iteration. This operator links the transmission conditions of all the time slices, allowing to solve the problem on all time slices in the same time using the Aitken acceleration of the convergence. Some perspectives of this work are given in the conclusion.

2 What are the right T.C. in the nonlinear case?

Let us first give a new formulation of the equation (2) assuming that $f(t,y(t)$ is scalar and $f^{-1}(t,y(t))$ exists. Then one can consider the problem:

$$-\frac{d}{dt}[-f^{-1}(t,y(t))\frac{d}{dt}y(t)] = -\frac{d}{dt}(-1) = 0, \, t \in]0,T[, y(0) = 0, \tag{3a}$$

$$y(T) = 1. \tag{3b}$$

where we imposed a Dirichlet B.C. at the time $t = T$ for the sake of simplicity. Then the multiplicative Schwarz with Neumann (associated to the Laplacian operator)-Dirichlet T.C. applied to $[0,T] = [0,1] = [0,\Gamma] \cup [\Gamma,1]$ with $\Gamma = 3/5$ writes:

$$-\frac{d}{dt}[-f^{-1}(t,y_1^{n+\frac{1}{2}}(t))\frac{d}{dt}y_1^{n+\frac{1}{2}}(t)]=0,\ t\in]0,\Gamma[,y_1^{n+\frac{1}{2}}(0)=0, \tag{4a}$$

$$y_1^{n+1}(\Gamma)=\alpha^n=y_2^n(\Gamma), \tag{4b}$$

and

$$-\frac{d}{dt}[-f^{-1}(t,y_2^{n+1}(t))\frac{d}{dt}y_2^{n+1}(t)]=0,\ t\in]\Gamma,1[,y_2^{n+1}(1)=1, \tag{5a}$$

$$\frac{d}{dt}y_2^{n+1}(\Gamma)=\beta^{n+1}=\frac{d}{dt}y_1^{n+\frac{1}{2}}(\Gamma). \tag{5b}$$

Let us consider $f(t,y(t))=\sqrt{y(t)}$ then the exact solution is $y(t)=t^2$ and $y(3/5)=\bar{\alpha}=9/25$. The exact solution of the Neumann-Dirichlet writes:

$$y_1^{n+\frac{1}{2}}(t)=\frac{25}{9}t^2\alpha^n\rightarrow\frac{d}{dt}y_1^{n+1}(\frac{3}{5})=\frac{10}{3}\alpha^n. \tag{6}$$

$$y_2^{n+1}(t)=\begin{cases}\frac{25}{4}r_1^2t^2+\frac{5}{2}r_1t(-5r_1-2)+\frac{1}{4}(-5r_1-2)^2,\\ \frac{25}{4}r_2^2t^2+\frac{5}{2}r_2t(-5r_2+2)+\frac{1}{4}(-5r_2+2)^2.\end{cases} \tag{7}$$

where r_1 (respectively r_2) is the root of $3r_1^2+3r_1+2\alpha=0$ (respectively $3r_2^2-r_2+2\alpha=0$). The sequence (α^n) satisfies one of the equation that follows:

$$\alpha^{n+1}=\begin{cases}f_1(\alpha^n)=1/2-(1/6)\sqrt{9-24\alpha^n}-(2/3)\alpha^n,\\ f_2(\alpha^n)=1/2+(1/6)\sqrt{9-24\alpha^n}-(2/3)\alpha^n.\end{cases} \tag{8}$$

If $\alpha^{n+1}=f_1(\alpha^n)$ then the sequence converges toward the fixed point $\bar{\alpha}_1=f_1(\bar{\alpha}_1)=0$ as $|f_1^{(1)}(\bar{\alpha}_1)|<1$. But $\bar{\alpha}_1\neq\bar{\alpha}$. If $\alpha^{n+1}=f_2(\alpha^n)$ then $\bar{\alpha}_2=f_2(\bar{\alpha}_2)=\bar{\alpha}$, but $|f_2^{(1)}(\bar{\alpha}_2)|>1$ and the function is not contractive. In both cases the multiplicative Schwarz will not converge with these transmission conditions.

If we replace Equation (5b) by Equation (9b):

$$-\frac{d}{dt}[-f^{-1}(t,y_2^{n+1}(t))\frac{d}{dt}y_2^{n+1}(t)]=0,\ t\in]\Gamma,1[,y_2^{n+1}(1)=1, \tag{9a}$$

$$f^{-1}(\Gamma,y_2^{n+1}(\Gamma))\frac{d}{dt}y_2^{n+1}(\Gamma)=\beta^{n+1}=f^{-1}(\Gamma,y_1^{n+\frac{1}{2}}(\Gamma))\frac{d}{dt}y_1^{n+\frac{1}{2}}(\Gamma). \tag{9b}$$

The sequence (α^n) of the Dirichlet condition satisfies :

$$\alpha^{n+1}=\begin{cases}0, \quad \alpha^n>\frac{9}{4},\\ \frac{4}{9}\alpha^n-\frac{4}{3}\sqrt{\alpha^n}+1, \quad 0\le\alpha^n<\frac{9}{4}.\end{cases}\ ,\text{thus}\ \ \alpha^n\rightarrow\overline{\alpha}=\frac{9}{25}.$$

This result shows that we can not simplify the T.C. by only taking the matching of the time derivatives between time slices, even if the nonlinear function $f^{-1}(t,y(t))$ is continuous.

Coming back to the original formulation of the Schwarz algorithm for the second order ODE Equation (2), the T.C. to replace the transmission condition $\frac{d}{dt}y_1^{m+\frac{1}{2}}(T^-) = \frac{d}{dt}\bar{y}_1^m(T^-)$ should be the flux or co-normal derivative $f^{-1}(y_1^{m+\frac{1}{2}}(T^-))\frac{d}{dt}y_1^{m+\frac{1}{2}}(T^-) = -f^{-1}(\bar{y}_1^m(T^-))\frac{d}{dt}\bar{y}_1^m(T^-)$, if $f^{-1}(y_1^{n+1}(T^-)) \neq 0$, else $\frac{d}{dt}y_1^{m+\frac{1}{2}}(T^-) = 0$. Moreover, this invariant of the problem, allows us to simplify the methodology too. We can impose (with assuming $f^{-1}(T^-,y(T^-)) \neq 0$) the B.C. $f^{-1}(T^-,y(T^-))\frac{d}{dt}y_(T^-) = 1$. Consequently, we do not need to symmetrize the time interval and then saving by a factor 2 the computational resources needed.

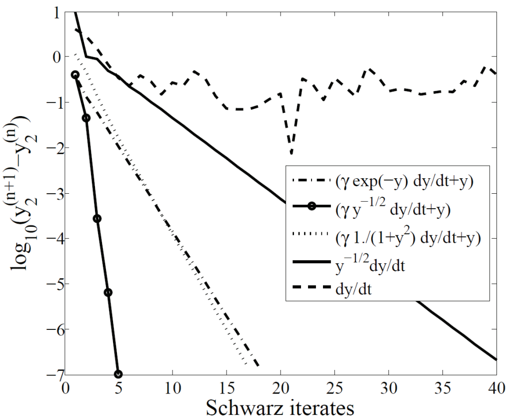

Fig. 1 Convergence/Divergence of the multiplicative Schwarz with respect to the T.C. $f^{-1}(t,y(t))\frac{d}{dt}y(t)$ with $f^{-1}(t,y(t)) = \{(\sqrt{y(t)})^{-1}, exp(-y(t)), \frac{1}{1+y^2(t)}\}$, or $\frac{d}{dt}y(t)$.

Figure 1 represents the numerical convergence of multiplicative Schwarz with the discretized nonlinear T.C. for the discretizing scheme associated to the Equation (3) with $f^{-1}(t,y(t)) = \{(\sqrt{y(t)})^{-1}, exp(-y(t)), \frac{1}{1+y^2(t)}\}$. It exhibits that the convergence behavior is purely linear for this problem with two time slices and one artificial interface. The T.C. with imposing the matching of $\frac{dy}{dt}(t)$ only does not converge as expected by the theory. The combining of the Dirichlet and relaxed flux for T.C. converges faster. We show in section 3 the pure linear behavior for the convergence of the multiplicative Schwarz for the time decomposition with this kind of nonlinear T.C. .

3 Pure linear convergence of the Time Schwarz DDM with nonlinear flux transmission conditions

Let us consider the problem Equation (3a) with Dirichlet B.C. at $t = 0$ and the invariant flux B.C. equal to 1 at $t = T$. Then we split the time interval $[0, T[$ into p time slices of size $H = T/p$ and we apply the multiplicative Schwarz algorithm with Dirichlet B.C. at $t = T_{i-1}^{+}$ and a combination of a Dirichlet and the invariant flux B.C. at $t = T_i^{-}$ times a parameter γ:

$$\frac{d}{dt} f^{-1}(t, y_i^{n+\frac{1}{2}}(t)) \frac{d}{dt} y_i^{n+\frac{1}{2}}(t) = 0, t \in S_i, \tag{10a}$$

$$y_i^{n+\frac{1}{2}}(T_{i-1}^{+}) = y_{i-1}^{n}(T_{i-1}^{-}), \tag{10b}$$

$$y_i^{n+\frac{1}{2}}(T_i^{-}) + \gamma f^{-1}(T_i^{-}, y_i^{n+\frac{1}{2}}(t)) \frac{d}{dt} y_i^{n+\frac{1}{2}}(T_i^{-}) = y_{i+1}^{n}(T_i^{+}) + \gamma f^{-1}(T_i^{+}, y_{i+1}^{n}(T_i^{+})) \frac{d}{dt} y_{i+1}^{n}(T_i^{+}). \tag{10c}$$

Following the idea of [2], we use the Kirchoff transformation by introducing new variables $u_i(t)$ such that

$$u_i(t) := \Theta(y_i(t)) = \int^{y_i(t)} f^{-1}(t, z(t)) dz \text{ a.e. in } S_i. \tag{11}$$

Then $f^{-1}(t, y_i(t)) \frac{d}{dt} y_i(t) = \frac{d}{dt} u_i(t)$. Here the $f^{-1}(t, z(t))$ is taken sufficiently continuous such that the value of $\Theta(y(t^{-})) = \Theta(y(t^{+}))$ and an equality on “y” traduces an equality on “u”. Schwarz Algorithm (10) can be rewritten as:

$$\frac{d^2}{dt^2} u_i^{n+\frac{1}{2}}(t) = 0, t \in S_i, \tag{12a}$$

$$u_i^{n+\frac{1}{2}}(T_{i-1}^{+}) = \eta_i^n \stackrel{def}{=} u_{i-1}^{n}(T_{i-1}^{-}), \tag{12b}$$

$$u_i^{n+\frac{1}{2}}(T_i^{-}) + \gamma \frac{du_i^{n+\frac{1}{2}}}{dt}(T_i^{-}) = \chi_i^n \stackrel{def}{=} u_{i+1}^{n}(T_i^{+}) + \gamma \frac{du_{i+1}^{n}}{dt}(T_i^{+}). \tag{12c}$$

We can show that the B.C. of this multiplicative Schwarz converge purely linearly to the B.C. associated to the solution. The error $e_i = u_i - u$ satisfies

$$\frac{d^2}{dt^2} e_i^{n+\frac{1}{2}}(t) = 0, t \in S_i, \tag{13a}$$

$$e_i^{n+\frac{1}{2}}(T_{i-1}^{+}) = e_{i-1}^{n}(T_{i-1}^{-}) = \alpha_i^n \stackrel{def}{=} \eta_i^n - \eta_i^{\infty}, \tag{13b}$$

$$e_i^{n+\frac{1}{2}}(T_i^{-}) + \gamma \frac{de_i^{n+\frac{1}{2}}}{dt}(T_i^{-}) = e_{i+1}^{n}(T_i^{+}) + \gamma \frac{de_{i+1}^{n}}{dt}(T_i^{+}) = \beta_i^n \stackrel{def}{=} \chi_i^n - \chi_i^{\infty}. \tag{13c}$$

The error $e_i(t)$ writes $e_i(t) = a_i\, t + b_i$ with:

$$a_i = \frac{\beta_i^n - \alpha_i^n}{\gamma + H}, \text{ and } b_i = -\frac{(\beta_i^n - \alpha_i^n)}{\gamma + H} T_{i-1}^{+} + \alpha_i^n. \tag{14}$$

For the sake of simplicity, let us take $p = 6$. We have $\alpha_1^n = 0$ and $\beta_6^n = 0$. Then one can write: $\Xi_1^{n+\frac{1}{2}} := (\beta_1^{n+\frac{1}{2}}, \alpha_3^{n+\frac{1}{2}}, \beta_3^{n+\frac{1}{2}}, \alpha_5^{n+\frac{1}{2}}, \beta_5^{n+\frac{1}{2}})^T = \mathbb{P}_1 \Xi_2^n$
and $\Xi_2^n := (\alpha_2^n, \beta_2^n, \alpha_4^n, \beta_4^n, \alpha_6^n)^T = \mathbb{P}_2 \Xi_1^{n-\frac{1}{2}}$ with:

$$\mathbb{P}_1 = \frac{1}{\gamma + H} \begin{pmatrix} -1 & 1 & 0 & 0 & 0 \\ \gamma & H & 0 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 \\ 0 & 0 & \gamma & H & 0 \\ 0 & 0 & 0 & 0 & -1 \end{pmatrix} \text{ and } \mathbb{P}_2 = \frac{1}{\gamma + H} \begin{pmatrix} H & 0 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & \gamma & H & 0 & 0 \\ 0 & 0 & 0 & -1 & 1 \\ 0 & 0 & 0 & \gamma & H \end{pmatrix}. \tag{15}$$

The matrices $\mathbb{P}_1$ and $\mathbb{P}_2$ do not depend on the iteration n, and are invertible with an appropriate choice of γ. The matrix $\mathbb{P} = \mathbb{P}_1 \mathbb{P}_2$ links all the B.C. associated to the odd time slices as follows:

$$\mathbb{P} = \frac{1}{(\gamma + H)^2} \begin{pmatrix} -H & -1 & 1 & 0 & 0 \\ \gamma H & -H & H & 0 & 0 \\ 0 & -\gamma & -H & -1 & 1 \\ 0 & \gamma^2 & \gamma H & -H & H \\ 0 & 0 & 0 & -\gamma & -H \end{pmatrix}. \tag{16}$$

Consequently the multiplicative Schwarz algorithm converges or diverges purely linearly and the right B.C. associated with the solution can be extrapolated with the Aitken's acceleration of convergence technique using this convergence or divergence behavior. By setting $\Lambda_1^{n+\frac{1}{2}} \stackrel{def}{=} (\chi_1^{n+\frac{1}{2}}, \eta_3^{n+\frac{1}{2}}, \chi_3^{n+\frac{1}{2}}, \eta_5^{n+\frac{1}{2}}, \chi_5^{n+\frac{1}{2}})^T$, the Aitken's extrapolation, with the identity matrix $\mathbb{I}$, writes: $\Lambda_1^{\infty} = (\mathbb{I} - \mathbb{P})^{-1}(\Lambda_1^{\frac{3}{2}} - \mathbb{P}\Lambda_1^{\frac{1}{2}})$. For $H = 1$ and $\gamma = 0.5$ the eigenvalues of $\mathbb{P}$ are with 4 significant digits:
$\{-0.1413 \pm 0.2478\,i, -0.2608, -0.2221 \pm 0.1496\,i\}$ which shows the convergence of the multiplicative Schwarz.

Remark 1. We can not impose the flux T.C. only at the end of time slices because the flux B.C. at the last time slices then will impose $a_i = 0, \forall i$. Consequently we would have a sequential propagation of the right B.C. at each Schwarz iterate.

Remark 2. As we have $\frac{d}{dt} u_{i+1}^n(T_i^+) = 1$ then Equation (10c) can be replaced by:

$$u_i^{n+\frac{1}{2}}(T_i^-) + \gamma \frac{d}{dt} u_i^{n+\frac{1}{2}}(T_i^-) = \chi_i^n \stackrel{def}{=} u_{i+1}^n(T_i^+) + \gamma. \tag{17}$$

4 Numerical implementation and result

In order to implement the multiplicative Schwarz, we still use Equation (2a) with using the Störmer-Verlet second order in time implicit scheme. Considering $N+1$ regular time steps Δt on each time slice S_i, and $z_j \simeq y_i(T_{i-1}^{+} + j\Delta t)$, the flux T.C. given by Equation (17) is discretized in time with the second order scheme with $f_N^{-1} = f(T_i^-, z_N)^{-1}$:

$$y_i(T_i^-) + \gamma f(T_i^-, y_i(T_i^-))^{-1} \frac{dy_i}{dt}(T_i^-) \simeq z_N + \gamma f_N^{-1}(\frac{3}{2}z_N - 2z_{N-1} + \frac{1}{2}z_{N-2}). \quad (18)$$

The local problem on each time slice consists in searching the zero of the function $F(z_0, \dots, z_N) = 0$ including the two T.C. for $j = 0$ and $j = N$ with a Newton method with a stopping criterion set to be 10^{-7}. The Jacobian matrix of F is mainly a tridiagonal matrix when we applied a Gaussian elimination of the term in position $N, N-2$. Moreover the nonlinearity is concentrated in the scheme only on the diagonal of the Jacobian and on the last row. An initial solution is computed on a regular coarse time mesh with the Newton stopping criterion set to be 9.10^{-2}. Then the Kirshoff transformation Θ is applied to the T.C. Y^i (of odd time slices) in order to obtain the acceleration matrix $\mathbb{P}_\Theta$. Next, the Aitken acceleration is performed in the transformed space (associated to the Kirshoff transformation) and the accelerated T.C. Y^∞ on odd time slices are retrieved with applying Θ^{-1} as follows:

$$Y^\infty := \Theta^{-1}\big((\mathbb{I} - \mathbb{P}_\Theta)^{-1}(\Theta(Y^2) - \mathbb{P}_\Theta \Theta(Y^1))\big). \quad (19)$$

Remark 3. This formula generalizes to the nonlinear case the Aitken-SVD [9]. In this last case, $\Theta(Y) = \mathbb{U}Y$ is the linear change of variable where $\mathbb{U}$ comes from the singular value decomposition $\mathbb{U}\Sigma\mathbb{V}^T$ of the T.C. arizing in the Schwarz iterations.

5 Conclusion

We obtained new nonlinear transmission conditions for our time domain decomposition which consists to apply classical multiplicative Schwarz algorithm on non-overlapping time slices. These T.C. make the multiplicative Schwarz algorithm having a pure linear convergence that allows it to be extrapolated to the T.C. satisfied by the searched solution. The method is for the moment applied to scalar problem, some extension to system of non linear ODEs is under investigation by using the definition of the inverse of a vector used in the ε-algorithm.

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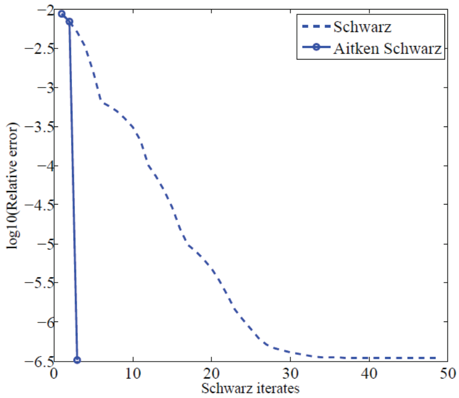

Fig. 2 Maximum of relative error between the Schwarz Dirichlet B.C. of odd time slices with the exact solution (dash line) and its acceleration by Aitken technique (solid line), with respect to the Schwarz iterations for $f(t,y(t)) = exp(y(t))$. Number of time slices is $p = 12$, $N = 81$, $\gamma = 20$.

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