On the links between observed and theoretical convergence rates for Schwarz waveform relaxation algorithm for the time-dependent problems

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Abstract In the framework of linear problems, a usual approach to study the convergence of Schwarz algorithms is to calculate the convergence rate in the frequency domain. However, for time-dependent problems, this tool provides results not fully representative of the observed behaviour of the algorithm. In this article we highlight differences between the theoretical convergence rate ρ and the convergence observed in the physical space-time domain. We also explain how the theoretical convergence rate can be used to provide bounds to the observed convergence rate ρ^{obs}. For problems defined on time windows of finite size, we recall that the bounds usually considered to study the convergence are empirical estimates albeit robust. In conclusion of this paper, numerical experiments are carried out to illustrate the relevance of the theoretical analysis.

1 Context

We study the application of Schwarz waveform relaxation algorithm for the time-dependent problem to a linear multiphysics problem on two non-overlapping physical domains Ω_1 and Ω_2:

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$$\begin{cases} \partial_t u_j(x,t) - \mathcal{A}_j u_j(x,t) = F_j(x,t) & \text{on } \Omega_j \times]0,T[\\ \mathcal{B}_j u_j(x,t) = G_j(x,t) & \text{on } \partial\Omega_j^{\text{ext}} \times]0,T[\\ u_j(x,0) = u_{j,0}(x) & \text{in } \Omega_j \end{cases} \tag{1a}$$

$$\begin{cases} C_{1,1} u_1|_\Gamma(t) = C_{1,2} u_2|_\Gamma(t) & \text{on } [0,T[\\ C_{2,2} u_2|_\Gamma(t) = C_{2,1} u_1|_\Gamma(t) & \text{on } [0,T[\end{cases} \tag{1b}$$

where T can be a finite or infinite time. The Schwarz waveform relaxation algorithm is applied on problem (1a) with interface conditions (1b). For given first guess $u_j^0|_\Gamma(t)$ on the interface Γ, the state of the algorithm is given at each iteration $n \in \mathbb{N}$ by (2). We suppose here the well-posedness of the initial problem (1) and of the algorithm (2). This means there exist a unique solution to (1) in $\mathcal{L}^2(0,T;\mathcal{L}(\Omega_j))$ noted $\widetilde{u}$ and there exist a unique $u_j^n \in \mathcal{L}^2(0,T;\mathcal{L}^2(\Omega_j))$ for all iterations n [1] . Some results on the well-posedness of such kind of problems can be found in [1, 2] (for problems on finite time window) and in a more general framework in [3] (for problems on finite or infinite time window).

$$\begin{cases} \partial_t u_1^n(z,t) - \mathcal{A}_1 u_1^n(x,t) = F_1(x,t) & \text{on } \Omega_1 \times [0,T[\\ \mathcal{B}_1 u_1^n(x,t) = G_1(x,t) & \text{on } \partial\Omega_1^{\text{ext}} \times [0,T[\\ u_1^n(x,0) = u_{1,0}(x) & \text{in } \Omega_1 \\ C_{1,1} u_1^n(x,t) = C_{1,2} u_2^{n-1}(x,t) & \text{on } \Gamma \times [0,T[\end{cases} \tag{2a}$$

$$\begin{cases} \partial_t u_2^n(x,t) - \mathcal{A}_2 u_2^n(x,t) = F_2(x,t) & \text{on } \Omega_2 \times [0,T[\\ \mathcal{B}_2 u_2^n(x,t) = G_2(x,t) & \text{on } \partial\Omega_2^{\text{ext}} \times [0,T[\\ u_2^n(x,0) = u_{2,0}(x) & \text{in } \Omega_2 \\ C_{2,2} u_2^n(x,t) = C_{2,1} u_1^n(x,t) & \text{on } \Gamma \times [0,T[\end{cases} \tag{2b}$$

From now on we also suppose $u_j^n(x) \in \mathcal{L}^2(]0,T[)$ for all $x \in \Omega_j$ [2]. To quantify and possibly optimize the convergence of algorithm (2), it is relevant to calculate a convergence rate as $\rho^{\text{obs}}_{\mathcal{A}_{\{1,2\}},\mathcal{B}_{\{1,2\}},C_{\{\{1,2\},\{1,2\}\}},j,n} = \left\|e_j^n\right\| / \left\|e_j^{n-1}\right\|$, where $e_j^n = u_j^n - \widetilde{u}|_{\Omega_j}$ is the error at each iteration n. In the rest of the paper, indicies $_{\mathcal{A},\mathcal{B},C}$ are neglected to simplify the notation.

Remark 1 We consider from now on that Ω_j are one-dimensional domains. Since all convergence factors are calculated in Fourier space, all results explained here can be extended to higher space dimensions parallel to the interface[3]. Also, we consider here Schwarz algorithms applied to multiphysics problems (for nonoverlapping domains) but the following results are also valid in the presence of an overlap.

[1] For example, for parabolic problems we need to have $F \in \mathcal{L}^2(0,T;\mathcal{L}^2(\Omega_j))$ and $u_{j,0} \in \mathcal{L}^2(\Omega_j)$

[2] For example, for parabolic problems we need to have $u_j^n \in \mathcal{L}^2(0,T;\mathcal{H}^1(\Omega_j))$, that it satisfied if G_j and first guess are regular enouth (see [4])

[3] This involves applying Fourier transforms in all directions parallel to the interface. Fourier transforms on spatial dimensions do not give rise to the problem that we expose here which is specific to the temporal dimension

2 Convergence for problems on an infinite time window

We first consider that the simulation is made on an infinite time window, i.e. $T = +\infty$.

Convergence factor in Fourier space: For time-dependent problems, the observed convergence factor cannot be calculated analytically. Thus a usual approach consists in applying a time Fourier transform to the error system. In the case where $T = +\infty$ and considering that the error is equal to zero for negative times, the convergence is determined in the Fourier space by solving the following system:

$$\begin{cases} i\omega\, \widehat{e}_1^n(x,\omega) - \mathcal{A}_1 \widehat{e}_1^n(z,\omega) = 0 & \text{on } \Omega_1 \times \mathbb{R} \\ \mathcal{B}_1 \widehat{e}_1^n(x,\omega) = 0 & \text{on } \partial\Omega_1^{ext} \times \mathbb{R} \\ C_{1,1}\widehat{e}_1^n(x,\omega) = C_{1,2}\widehat{e}_2^{n-1}(x,\omega) & \text{on } \Gamma \times \mathbb{R} \end{cases} \tag{3a}$$

$$\begin{cases} i\omega \widehat{e}_2^n(x,\omega) - \mathcal{A}_2 \widehat{e}_2^n(x,\omega) = 0 & \text{on } \Omega_2 \times \mathbb{R} \\ \mathcal{B}_2 \widehat{e}_2^n(x,\omega) = 0 & \text{on } \partial\Omega_2^{ext} \times \mathbb{R} \\ C_{2,2}\widehat{e}_2^n(x,\omega) = C_{2,1}\widehat{e}_1^n(x,\omega) & \text{on } \Gamma \times \mathbb{R} \end{cases} \tag{3b}$$

Suppose that (3) can be solved for any $\omega \in \mathbb{R}$, then the convergence factor ϱ and convergence rate ρ in the Fourier space can be calculated as:

$$\varrho(\omega) := \frac{\widehat{e}_j^n|_\Gamma(\omega)}{\widehat{e}_j^{n-1}|_\Gamma(\omega)} \qquad \rho(\omega) := |\varrho(\omega)| \tag{4}$$

It can be shown that ρ is independent of the space variable x and of the domain j. Without lack of generality, from now on suppose ρ is calculate from the errors at the interface Γ. General methods to study the convergence of Schwarz algorithms can be found in [5, 6, 7].

Observed convergence factor: From the well-posedness properties of the algorithm, we assume that $e_j^n(x,\cdot) \in \mathcal{L}^2(\mathbb{R})$ for all $x \in \Omega_j$. Then $\widehat{e}_j^n(x,\cdot) \in \mathcal{L}^2(\mathbb{R})$ and the following inequality is obviously satisfied:

$$\inf_{\omega\in\mathbb{R}} \rho(\omega) \left\|\widehat{e}_j^{n-1}(x,\cdot)\right\|_2 \le \left\|\widehat{e}_j^n(x,\cdot)\right\|_2 \le \sup_{\omega\in\mathbb{R}} \rho(\omega) \left\|\widehat{e}_j^{n-1}(x,\cdot)\right\|_2 \tag{5}$$

Thanks to Parseval's theorem, we can thus provide the following bounds to the observed convergence factor:

$$\inf_{\omega\in\mathbb{R}} \rho(\omega) \le \frac{\left\|e_j^n(x,\cdot)\right\|_2}{\left\|e_j^{n-1}(x,\cdot)\right\|_2} =: \rho_{j,n}^{\text{obs}}(x) \le \sup_{\omega\in\mathbb{R}} \rho(\omega)\,. \tag{6}$$

Thus, if $\sup_{\omega\in\mathbb{R}} \rho(\omega) < 1$ then algorithm (2) converges in $\mathcal{L}^2(]0,+\infty[)$ norm : $\|e_j^n(x,\cdot)\|_2 \xrightarrow[n\to\infty]{} 0$. Moreover, because ρ given by (4) is the same for all $x \in \Omega_j$, previ-

ous bounds (5) and (6) are also valid for $\rho^{\text{obs}}_{j,n} := \left\|e^n_j\right\|_{\mathcal{L}^2(]0,\infty[,\mathcal{L}^2(\Omega))} / \left\|e^{n-1}_j\right\|_{\mathcal{L}^2(]0,\infty[,\mathcal{L}^2(\Omega))}$. Finally the theoretical convergence rate ρ provides bounds for the observed convergence in the $\mathcal{L}^2(]0,\infty[,\mathcal{L}^2(\Omega_j))$ norms.

Discrete in time problems : Let first assume that we simulate the semi-discrete problem over an infinite time window with a similar time step δt in both subdomains. The observed numerical error is denoted $E^{n,m}_j(x)$ with $m \in \mathbb{N}$, and can be seen as the result of a Dirac comb on the continuous error $e^n_j(x,\cdot)$:

$$E^{n,m}_j(x) = U^{n,m}_j(x) - u(x,t^m) \qquad \text{and} \qquad E^{n,\cdot}_j(x) = \Delta_{\delta t} e^n_j(x,\cdot)$$

with U the solution of the discrete problem, $\Delta_{\delta t}$ the Dirac comb of period δt and $e^n_j(x,t)$ the error on the continuous problem.[4] Frequencies higher than $\pi/\delta t$ are not generated by the temporal grid [8]. Applying Shannon theorem leads to restrict the study of the errors in Fourier space $\widehat{E^{n,\cdot}_j}$ on an interval $I_\omega := \left[-\frac{\pi}{\delta t}; \frac{\pi}{\delta t}\right]$ and $\widehat{E^{n,\cdot}_j}(x,\omega) = \widehat{e^n_j}(x,\omega)$ for all $\omega \in I_\omega$. Details of the process can be found in [9]. Thus $\mathcal{L}^2$ norm of $\widehat{E^{n,\cdot}_j}$ can be calculate using result of the continuous case. Parseval's theorem can be used to obtain bounds on observed convergence rate in $\mathcal{L}^2$ norm:

$$\min_{|\omega|\le\pi/\delta t} \rho(\omega) \le \rho^{\text{obs}}_{j,n}(x) := \frac{\left\|E^{n,\cdot}_j(x)\right\|_2}{\left\|E^{n-1,\cdot}_j(x)\right\|_2} \le \max_{|\omega|\le\pi/\delta t} \rho(\omega) \tag{7}$$

Consequently, the same bounds apply on convergence rate $\rho^{\text{obs}}_{j,n}$ in $\mathcal{L}^2(]0,\infty[,\mathcal{L}^2(\Omega_j))$ norm.

3 Convergence for problems on a finite time window

Bold notation is used to describe the solution $\mathbf{u}^n_j$ and the error $\mathbf{e}^n_j$ over a finite window of time $[0,T]$ with $0 < T < +\infty$. We will consider $\omega \in I_\omega$ with $I_\omega = \mathbb{R}$ if we consider a continuous simulation, and I_ω defined in section 2 if we consider a discrete problem.

Difficulties expressing error over a finite time window: Applying the Fourier transform to the windowed signal would lead to search for the solution of an equation of the type:

$$i\omega\widehat{\mathbf{e}}^n_j(x,\omega) + \mathcal{A}(\widehat{\mathbf{e}}^n_j(x,\omega)) = -\mathbf{e}^n_j(x,T)\exp(-i\omega T) \tag{8}$$

[4] Here the discrete solution U (resp. the discrete error E) is obtained by discretizing the continuous solution u (resp. the continous error e). The discrete signal optained with a numerical simulation is an approximation of U depending on the numerical scheme.

Without more knowledge about the error at time T, one cannot solve the differential equation (8), therefore cannot express the error $\widehat{\mathbf{e}}_j^n(z,\omega)$ according only to the parameters of the equation. Nevertheless, the error can be expressed by $\widehat{\mathbf{e}} = \widehat{e} * \widehat{P}_{[0,T]}(\omega)$ where P is the rectangular function on $[0,T]$ and $\widehat{P}_{[0,T]} = T\exp(-i\omega T/2)\,\mathrm{sinc}(\omega T/2)$ The convergence rate for the error $\mathbf{e}$ for a given frequency ω thus reads:

$$\boldsymbol{\rho}(\omega) = \left|\frac{\widehat{e^{n+1}}|_\Gamma * \widehat{P_{[0,T]}}(\omega)}{\widehat{e^n}|_\Gamma * \widehat{P_{[0,T]}}(\omega)}\right| = \left|\frac{\int \varrho(\theta)\,\widehat{e^n}|_\Gamma(\theta)\widehat{P_{[0,T]}}(\omega-\theta)\,d\theta}{\int \widehat{e^n}|_\Gamma(\theta)\widehat{P_{[0,T]}}(\omega-\theta)\,d\theta}\right| \tag{9}$$

which clearly shows that ρ and $\boldsymbol{\rho}$ are different functions, except in the exceptional case where $\varrho(\omega)$ is a constant. Also, definition (9) supports that function ρ cannot be seen as the convergence factor at a given frequency: $\rho(\omega) \neq |\widehat{\mathbf{e}_j^n}(\omega)|/|\widehat{\mathbf{e}_j^{n-1}}(\omega)|$.

Bound on observed convergence : The bound on the convergence factor given by (9) is complicated to determined. However it is possible to directly bound the error :

Theorem 1 (Bound on the $\mathcal{L}^2$ norm)

$$\left\|\mathbf{e}_j^n(x,\cdot)\right\|_2 \leq \left(\sup_{\omega\in I_\omega}\rho(\omega)\right)^n \left\|\mathbf{e}_j^0(x,\cdot)\right\|_2 \tag{10}$$

wich implies a bound for the n-product on the observed convergence rate:

$$\prod_{k=1}^{n}\boldsymbol{\rho}_{j,k}^{obs}(x) \leq \left(\sup_{\omega\in I_\omega}\rho(\omega)\right)^n \qquad \forall x\in\Omega_j \tag{11}$$

This ensures the convergence of the error for the windowed algorithm as long as $\sup_{\omega\in I_\omega}\rho(\omega) < 1$. *This bounds also works for* $\left\|\mathbf{e}_j^n\right\|_{L(]0,T[,\mathcal{L}^2(\Omega_j))}$.

Proof It is possible to link the convergence of the windowed problem to a corresponding infinite-in-time problem. We can bound the $\mathcal{L}^2$ norm of error on the windowed problem by the corresponding error of a inifite in time problem : $\left\|\mathbf{e}_j^n(x,\cdot)\right\|_2 \leq \left\|e_j^n(x,\cdot)\right\|_2 \leq \left(\sup_{\omega\in I_\omega}\rho(\omega)\right)^n \left\|e_j^0(x,\cdot)\right\|_2$ where e_j^0 is any first guess extended to infinite time. Using the particular extension $e_j^0|_{[0,T]} = \mathbf{e}_j^0$ and $e_j^0|_{]T,\infty[} = 0$ leads to (10). Then combining $\|\mathbf{e}_j^n(x,\cdot)\|_2/\|\mathbf{e}_j^0(x,\cdot)\|_2 = \prod_{k=1}^{n}\boldsymbol{\rho}_{j,k}^{obs}(x)$ and (10) leads to (11). □

Remark 2 A bound on the convergence factor given by (9) was already calculated in [10]. This bound is complicated to calculate and then hardly usable. In this paper, a global remark on the possible influencing of the time windowing is done. It is

explained why the method used in [1, 11] needs special conditions and cannot be applied in a general context [5].

Range of influencing frequencies: For a given problem discretized in time δt over a time window $[0.T]$, we estimate that in the general framework:

$$\min_{\pi/T \leq |\omega| \leq \pi/\delta t} \rho(\omega) \leq \boldsymbol{\rho}_{j,n}^{\text{obs}}(x) \leq \max_{\pi/T \leq |\omega| \leq \pi/\delta t} \rho(\omega) \tag{12}$$

and the interval $|\omega| \in \left[\frac{\pi}{T}, \frac{\pi}{\delta t}\right]$ is called *influencing frequencies*. This interval of frequencies is usually considered for optimizing the convergence rate. As discussed in section 2, it is justified to consider that $\pi/\delta t$ is the maximum frequency. However the choice of the minimum frequency is justified only for time-independent problems but is an empirical estimate for time-dependent problems. We can still find justifications for this choice by considering the definition (9). First, it shows that convergence is influenced by $\int \rho(\theta) d\theta$ more than by its value at a given frequency ω. Moreover, thanks to the property of $\widehat{P}(\omega - \theta)$, frequencies such that $|\omega| \ll \pi/T$ have a low impact on the convergence[6]. That said, relevance of the minimum influncing frequency π/T is to be proved.

Remark 3 (minimal frequency for time-independent problem) The frequency $\omega_{\min}$ is justified in some cases of time-independent problem. If the conditions on border of the dimension parallel to the interface (the one where the Fourier transform is made) are determined, then the corresponding error system is periodic and a Discrete Fourier Transform (DFT) can be applied (for example see [12]). In our case, we can apply a Fourier transform on our discretised signal but, for the reasons evoked section 3, we cannot guarantee that $|DFT(\mathbf{e}_j^{n+1})(\omega_i)|/|DFT(\mathbf{e}_j^n)(\omega_i)|$ is equal to $\rho(\omega_i)$.

Remark 4 (optimization) Usually the optimisation of the convergence speed is made by choosing interface conditions $C_{\{\{1,2\},\{1,2\}\}}$ under such conditions C, such that $\inf_{C_{\{\{1,2\},\{1,2\}\}} \in C} \max_{\pi/T \leq |\omega| \leq \pi/\delta t} \rho_{C_{\{\{1,2\},\{1,2\}\}}}(\omega)$. From (12) this guarantee an minimal upper bound to the observed convergence rate and consequently a fast convergence of $\left\| e_j^n \right\|_{\mathcal{L}^2(0,T,\mathcal{L}^2(\Omega))}$ to zero.

4 Numerical illustration

We propose to illustrate the previous properties on the coupling of two diffusion equations, with Dirichlet-Neumann interface conditions with a non-overlapping interface in $x = 0$.

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[5] it requires the determination of the inverse Fourier transform $\left\|\mathcal{F}^{-1}\rho\right\|_1$ which may not exist or can be hard to calculate

[6] for a given ω, frequencies such that $|\omega - \theta| \ll \pi/T$ are drown in the integration in (9)

$$\begin{cases} \partial_t u_j(x,t) - \nu_j \partial_x^2 u_j(x,t) = 0 & \text{on } \Omega_j \times]0,T[\\ u_j(x,t) = 0 & \text{on } \partial\Omega_j^{\text{ext}} \times]0,T[\\ u_j(x,t=0) = 0 & \text{on } \Omega_j \end{cases} \tag{13a}$$

$$\begin{cases} u_1(0,t) = u_2(0,t) & \text{on } [0,T[\\ \nu_2 \partial_x u_2(0,t) = \nu_1 \partial_x u_1(0,t) & \text{on } [0,T[\end{cases} \tag{13b}$$

with $\Omega_1 = [h_1, 0]$ and $\Omega_2 = [0, h_2]$. We simulate the problem via an implicit finite difference scheme. Schwarz's algorithm on this problem is performed on 20 iterations, with a time step $\delta t = 1000$s and parameters $h_1 = -50$m, $h_2 = 300$m, $\nu_1 = 0.12\text{m}^2\text{s}^{-1}$ and $\nu_2 = 0.6\text{m}^2\text{s}^{-1}$. In figures 1 and 2 we compare the theoretical convergence rate given in the Fourier domain $\rho(\omega)$ with the observed convergence rate $\boldsymbol{\rho}_{n,j}^{obs}$ and the convergence rate measured on the DFT of the error at the interface $|DFT(\mathbf{e}_j^{n+1})(0,\omega_i)|/|DFT(\mathbf{e}_j^{n})(0,\omega_i)|$ which can be seen as an approximation of $\boldsymbol{\rho}(\omega_i)$. Fisrt guesses are initialised by a random signal which generates a large frequency spectrum. In these two figures, we find that bounds of the observed convergence verify the estimate (12) thus also verify theorem 1. The evolution of the $\mathcal{L}^2$ norm of the error is not explicitly given here but it can be deduce from $\boldsymbol{\rho}_{j,n}^{obs}$ (middle panel in 1 and 2). As expected the convergence observed on a given frequency ω_i does not correspond to the theoretical convergence $\rho(\omega_i)$ and conversely we tend towards equality for a window of assumed size infinite. Other examples on such problems were made in [13] and corroborate the estimate.

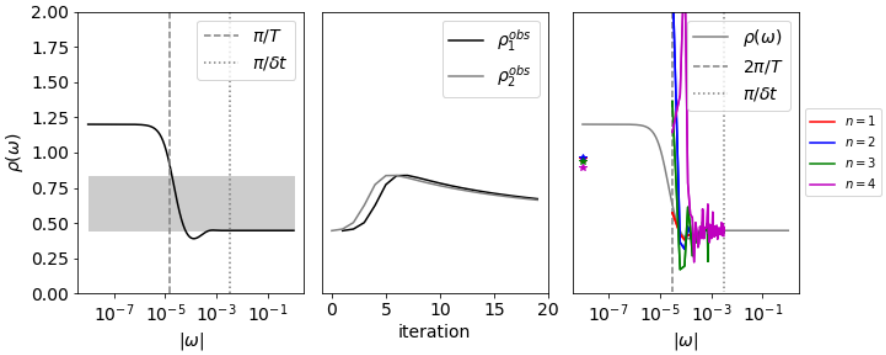

Fig. 1 For a finite time window with $T = 200\delta t$. Left panel: theoretical convergence rate $\rho(\omega)$, influencing frequencies are given by vertical lines and grey zones give the reached values of $\boldsymbol{\rho}_{j,n}^{\text{obs}}$. The observed convergence factor $\boldsymbol{\rho}_{j,n}^{\text{obs}}$ is given in the middle panel as a function of the iteration number n for the two domains. Right panel: the observed rate $|DFT(\mathbf{e}_1^n)(0,\omega_i)|/|DFT(\mathbf{e}_1^{n-1})(0,\omega_i)|$ is compared to the theoretical convergence rate ρ for the first four iterations.

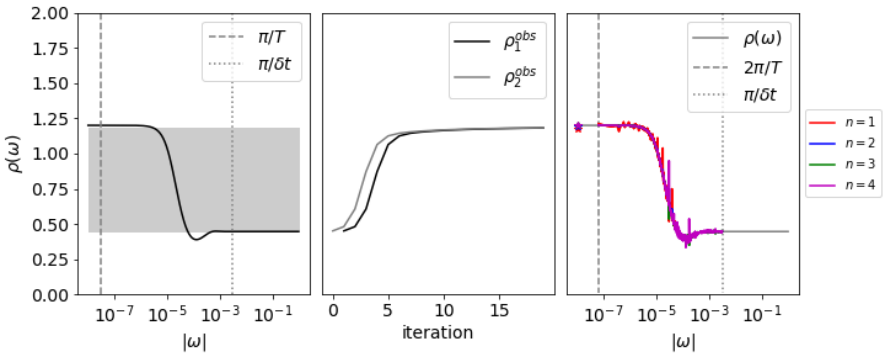

Fig. 2 Same as Figure 1 with $T = 10^5$. It is considered to be close to an infinite time window.

5 Conclusion

In the context of a time dependent problem, the convergence rate ρ calculated in the Fourier space can only be taken as such on problem considering an infinite time window. Thanks to Parceval theorem, informations on the algorithm in the physical space can be obtain on the $\mathcal{L}^2$ norm of the error. It is therefore possible to bound the observed convergence rate ρ^{obs} with the bounds of the theoretical convergence ρ. For a finite time window, we can no longer consider ρ as a convergence rate for a given frequency. Yet, bounds on the observed convergence rate are still relevant and we can precise these bounds by estimating an interval of influencing frequencies. In a futur work, it may be relevant to determine how to choose optimized interface conditions using the results on the observed convergence rate.

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