A time adaptive Neumann-Neumann waveform relaxation method for thermal fluid-structure interaction

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1 Introduction

Our prime motivation is thermal fluid-structure interaction (FSI) where two domains with jumps in the material coefficients are connected through an interface. There exist two main strategies to simulate FSI models: the monolithic approach where a new code is tailored for the coupled equations and the partitioned approach that allows to reuse existing software for each sub-problem. Here we want to develop multirate methods that contribute to the time parallelization of the sub-problems for the partitioned simulation of FSI problems.

We suggest here a parallel, time adaptive multirate method to solve two heterogeneous coupled heat equations which could be applied to FSI problems. The work to be presented is the time adaptive extension of the parallel multirate method in [13]. Some work has already been done regarding time adaptive multirate methods for the simulation of FSI problems. A time adaptive partitioned approach built over the Dirichlet-Neumann iteration for thermal FSI was presented in [4, 5]. In [11], two new iterative partitioned coupling methods that allow for the simultaneous execution of flow and structure solvers were introduced.

A new method that at each iteration solves the two subproblems simultaneously in parallel before exchanging information across the interfaces for the coupling of two parabolic problems was introduced in [10, 9, 6]. There, the Neumann-Neumann waveform relaxation (NNWR) method which is a waveform relaxation (WR) method based on the classical Neumann-Neumann iteration is described. It allows the use of different spatial and time discretizations for each subdomain. In [14],

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a pipeline implementation of the NNWR method together with its parallel efficiency is analyzed for the coupling of homogeneous materials. However, parallelization in time for the coupling of heterogeneous materials was not yet considered.

In a previous work [13], we proposed and analyzed a parallel multirate partitioned approach based on the NNWR algorithm [10, 9, 6] for two coupled parabolic problems with heterogeneous material coefficients. In this work, time adaptivity is added to the multirate approach resulting in a partitioned coupled scheme that allows at each iteration to find the local solutions of the subproblems over a certain time window using different time step controllers. In this setting, one does not need to exchange information across the interface after each time step. The numerical results show the advantages of the time adaptive method over the previous multirate approach.

2 Model problem

The unsteady transmission problem reads as follows, where we consider a domain $\Omega \subset \mathbb{R}^d$ which is cut into two subdomains $\Omega = \Omega_1 \cup \Omega_2$ with transmission conditions at the interface $\Gamma = \partial\Omega_1 \cap \partial\Omega_2$:

$$\begin{cases} \alpha_m \frac{\partial u_m(\mathbf{x},t)}{\partial t} - \nabla \cdot (\lambda_m \nabla u_m(\mathbf{x},t)) = 0, \ \ \mathbf{x} \in \Omega_m \subset \mathbb{R}^d, \ m = 1,2, \\ u_m(\mathbf{x},t) = 0, \ \ \mathbf{x} \in \partial\Omega_m \backslash \Gamma, \\ u_1(\mathbf{x},t) = u_2(\mathbf{x},t), \ \ \mathbf{x} \in \Gamma, \\ \lambda_2 \frac{\partial u_2(\mathbf{x},t)}{\partial \mathbf{n}_2} = -\lambda_1 \frac{\partial u_1(\mathbf{x},t)}{\partial \mathbf{n}_1}, \ \ \mathbf{x} \in \Gamma, \\ u_m(\mathbf{x},0) = u_m^0(\mathbf{x}), \ \ \mathbf{x} \in \Omega_m, \end{cases} \tag{1}$$

where $t \in [T_0, T_f]$ and $\mathbf{n}_m$ is the outward normal to Ω_m for $m = 1,2$.

The constants λ_1 and λ_2 describe the thermal conductivities of the materials on Ω_1 and Ω_2 respectively. D_1 and D_2 represent the thermal diffusivities of the materials and they are defined by

$$D_m = \frac{\lambda_m}{\alpha_m}, \ \text{ with } \ \alpha_m = \rho_m c_{p_m} \tag{2}$$

where ρ_m represents the density and c_{p_m} the specific heat capacity of the material placed in Ω_m, $m = 1,2$.

3 The Neumann-Neumann waveform relaxation algorithm

We now describe the Neumann-Neumann waveform relaxation (NNWR) algorithm [10, 9]. The main advantage of the NNWR method is that it allows to find the solution on the subdomains in parallel.

The NNWR algorithm starts by imposing continuity of the solution across the interface (i.e, given a common initial guess $g^0(\mathbf{x},t)$ on $\Gamma \times (T_0,T_f)$). One can then find the local solutions $u_m^{k+1}(\mathbf{x},t)$ on Ω_m, $m = 1,2$ through the following Dirichlet problems:

$$\begin{cases} \alpha_m \frac{\partial u_m^{k+1}(\mathbf{x},t)}{\partial t} - \nabla \cdot (\lambda_m \nabla u_m^{k+1}(\mathbf{x},t)) = 0, \ \ \mathbf{x} \in \Omega_m, \\ u_m^{k+1}(\mathbf{x},t) = 0, \ \ \mathbf{x} \in \partial\Omega_m \backslash \Gamma, \\ u_m^{k+1}(\mathbf{x},t) = g^k(\mathbf{x},t), \ \ \mathbf{x} \in \Gamma, \\ u_m^{k+1}(\mathbf{x},0) = u_m^0(\mathbf{x}), \ \ \mathbf{x} \in \Omega_m. \end{cases} \tag{3}$$

Now the second coupling condition which is the continuity of the heat fluxes is added. To this end, one solves two simultaneous Neumann problems to get the correction functions $\psi_m^{k+1}(\mathbf{x},t)$ on Ω_m, $m = 1,2$ where the Neumann boundary condition at the interface $\Gamma \times (T_0,T_f)$ is prescribed by the addition of the heat fluxes of the solutions $u_m^{k+1}(\mathbf{x},t)$ given by the Dirichlet problems:

$$\begin{cases} \alpha_m \frac{\partial \psi_m^{k+1}(\mathbf{x},t)}{\partial t} - \nabla \cdot (\lambda_m \nabla \psi_m^{k+1}(\mathbf{x},t)) = 0, \ \ \mathbf{x} \in \Omega_m, \\ \psi_m^{k+1}(\mathbf{x},t) = 0, \ \ \mathbf{x} \in \partial\Omega_m \backslash \Gamma, \\ \lambda_m \frac{\partial \psi_m^{k+1}(\mathbf{x},t)}{\partial \mathbf{n}_m} = \lambda_1 \frac{\partial u_1^{k+1}(\mathbf{x},t)}{\partial \mathbf{n}_1} + \lambda_2 \frac{\partial u_2^{k+1}(\mathbf{x},t)}{\partial \mathbf{n}_2}, \ \ \mathbf{x} \in \Gamma, \\ \psi_m^{k+1}(\mathbf{x},0) = 0, \ \ \mathbf{x} \in \Omega_m. \end{cases} \tag{4}$$

Finally, the interface values are updated with

$$g^{k+1}(\mathbf{x},t) = g^k(\mathbf{x},t) - \Theta(\psi_1^{k+1}(\mathbf{x},t) + \psi_2^{k+1}(\mathbf{x},t)), \ \ \mathbf{x} \in \Gamma, \tag{5}$$

where $\Theta \in (0,1]$ is the relaxation parameter. Note that if one uses the optimal relaxation parameter, we obtain a direct solver instead of an iterative method [6, 13].

In our previous work [13] we presented a multirate method for two heterogeneous coupled heat equations based on the NNWR algorithm. There, an interface interpolation that preserves a second order numerical solution of the coupled problem when using SDIRK2 was described to communicate data between the subdomains through the space-time interface in the multirate case. Furthermore, we performed a fully discrete one-dimensional analysis of the NNWR algorithm in (3)-(5) to find the optimal relaxation parameter in terms of the material coefficients, the time and space resolutions.

In this work we introduce a new adaptive scheme that, in contrast to the multirate method in [13], optimizes the total number of time steps for each subsolver allowing big step sizes without increasing the error of the numerical solution becoming a more efficient method.

4 Time adaptive method

We build our partitioned time adaptive approach on the SDIRK2-NNWR algorithm introduced in [12, chap.6] and in [13]. To that end, an error estimate at each time step is needed to be able to choose a new step size. In particular, we use an embedded technique [8, chap. IV.8].

In our approach, time adaptive processes for the time integration of the two Dirichlet problems (3) build two independent time grids τ_1 and τ_2. The Neumann problems (4) and the update step (5) then use these grids.

As our time adaptive SDIRK2-NNWR algorithm contains two time adaptive Dirichlet solvers, the corresponding local errors are given by the difference

$$\mathbf{r}_m^{n+1} = \mathbf{u}_I^{(m),n+1} - \hat{\mathbf{u}}_I^{(m),n+1}, \tag{6}$$

where $\mathbf{u}_I^{(m),n+1}$ and $\hat{\mathbf{u}}_I^{(m),n+1}$ are the two solutions of the embedded SDIRK2 method for $m = 1,2$ and n is the index of the time recursion. Taking the Euclidean norm throughout we consider the error estimate at each time step given by $\|\mathbf{r}_m^{n+1}\|_2$, $m = 1,2$. We then use a proportional-integral controller (PI controller) [15, 16],

$$\Delta t_m^{n+1} = \Delta t_m^n \left(\frac{TOL_m}{\|\mathbf{r}_m^{n+1}\|_2}\right)^{1/12} \left(\frac{TOL_m}{\|\mathbf{r}_m^{n}\|_2}\right)^{1/12}, \tag{7}$$

for the Dirichlet problem on the subdomain Ω_m for $m = 1,2$ respectively. Here we use the current error estimate, as well as the previous error estimate. However, on the first step $\mathbf{r}_m^0$ are not available and for that reason, we put $\mathbf{r}_m^0 = TOL_m$.

In order to start the integration, one also needs to pick an initial step size. Instead of using the classic result in [7, pp. 169], we use the following formula suggested by Gustaf Söderlind and inspired by [1, pp. 682-683]

$$\Delta t_m^0 = \frac{|T_f - T_0| \cdot TOL_m^{1/2}}{100 \cdot \left(1 + \|\mathbf{M}_{II}^{(m)^{-1}} \mathbf{A}_{II}^{(m)} \mathbf{u}_I^{(m),0}\|_2\right)}, \tag{8}$$

where $\mathbf{M}_{II}^{(m)}$ and $\mathbf{A}_{II}^{(m)}$ for $m = 1,2$ correspond to the mass and stiffness matrices of the finite element (FE) discretization respectively.

We have chosen the inner time adaptive tolerances finer than the outer tolerance used to terminate the iteration. Specifically, we take $TOL_m = TOL/5$ for $m = 1,2$. This choice is motivated by [17] and already used in a similar context in [3, sec. 6].

Finally, the relaxation parameter Θ in the update step (5) needs to be determined to ensure the efficiency of the whole algorithm. This issue is addressed in the next section.

5 Time adaptive relaxation parameter

In [13], we found the optimal relaxation parameter Θ_{opt} assuming structured spatial grids and conforming time grids on both subdomains in 1D using implicit Euler. Θ_{opt} is dependent on the coupled material coefficients α_1, α_2, λ_1, λ_2, the spatial resolution Δx and the time resolution Δt and the method using Θ_{opt} converges typically within two iterations. We then showed numerically that the nonmultirate 1D Θ_{opt} gives excellent estimates for the multirate case using SDIRK2 both in 1D and 2D.

The aim here is to adapt the formula derived for Θ_{opt} in [13] to the variable step size context. The main issues in the time adaptive approach are that we do not have a fixed value for Δt and we do not know beforehand how the time grids τ_1 and τ_2 look like. We propose to start the algorithm with an initial guess for Θ and update the value at each iteration once the time grids τ_1 and τ_2 have already been computed. Both the initial guess and the update to be presented are motivated by the numerical experiments shown in [13].

It has been observed in the non adaptive SDIRK2-NNWR scheme that the optimal relaxation parameter moves from one limit to the other in terms of the relation between Δt and Δx^2. Initially, as Δt is unknown because there is no fixed time step in the time adaptive framework, we suggest to take an intermediate value between the two limits. Although other options were tried as the geometric mean between the limits, the minimum or the maximum, the arithmetic mean was found to be the most efficient.

Firstly, the initial guess for the relaxation parameter Θ_0 is chosen as the arithmetic mean between the spatial and the temporal limits of Θ_{opt},

$$\Theta_0 := \frac{\alpha_1\alpha_2}{2(\alpha_1+\alpha_2)^2} + \frac{\lambda_1\lambda_2}{2(\lambda_1+\lambda_2)^2}. \tag{9}$$

Secondly, in order to update the relaxation parameter after each iteration, we average the obtained variable step sizes getting the means $\bar{\Delta t_1}$ and $\bar{\Delta t_2}$ for each space-time subdomain $\Omega_1 \times [T_0, T_f]$ and $\Omega_2 \times [T_0, T_f]$. Once we have the values $\bar{\Delta t_1}$ and $\bar{\Delta t_2}$ we choose Θ using the same strategy we presented in [13] for the non adaptive multirate SDIRK2-NNWR algorithm. There, we observe that one can use $\Theta_{opt}(\Delta t_2)$ when $\Delta t_1 < \Delta t_2$ and $\Theta_{opt}(\Delta t_1)$ when $\Delta t_1 > \Delta t_2$.

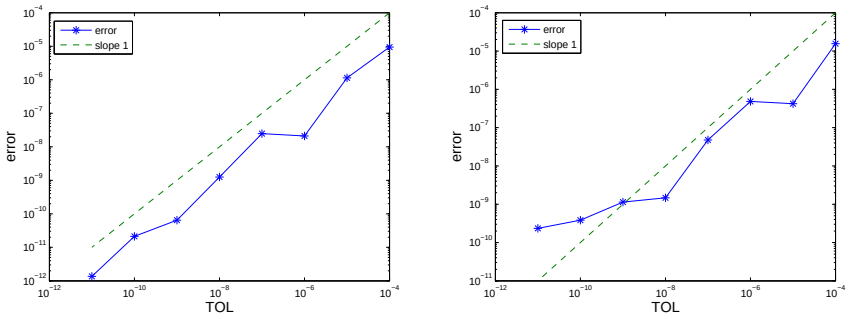
6 Numerical results

All the results in this section have been produced by implementing the algorithm in Python using the classical one-dimensional linear FE discretization on equidistant and identical meshes on both subdomains and using as a initial condition the smooth function $g(x) = 900(-x^2+2x)$ at the interval $\Omega = \Omega_1 \cup \Omega_2 = [0,1] \cup [1,2]$. Physical properties of the materials are shown in table 1.

Table 1 Physical properties of the materials. λ is the thermal conductivity, ρ the density, c_p the specific heat capacity and $\alpha = \rho c_p$.

Material	λ (W/mK)	ρ (kg/m^3)	c_p (J/kgK)	α (J/K m^3)
Air	0.0243	1.293	1005	1299.5
Water	0.58	999.7	4192.1	4.1908e6
Steel	48.9	7836	443	3471348

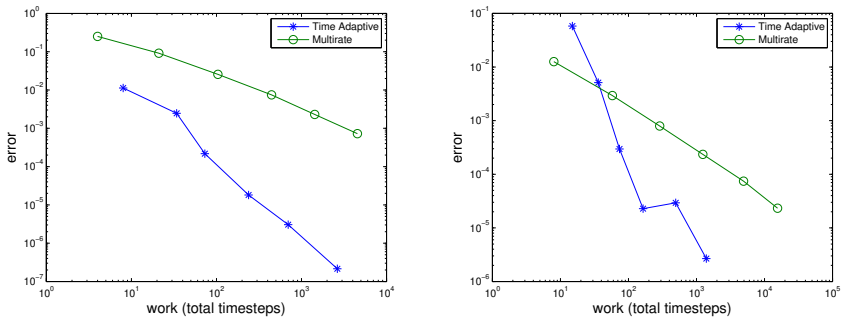
Figure 1 shows the global error of the overall solution on Ω with respect to the tolerance for the coupling of different materials. It has been calculated with respect to a reference solution u_{ref} that has been computed using the time adaptive SDIRK2-NNWR algorithm for a very fine tolerance ($TOL = 1e-12$). One observes in figure 1 how the error decreases proportionally to the tolerance as expected in a time adaptive numerical method. Some deviations are observed for the smallest tolerances in the coupling air-water. This could happen because the difference of the solution with respect to the reference at those points is not strong enough.



(a) *Air-steel* (b) *Air-water*

Fig. 1 Global error as a function of the tolerance of the time adaptive SDIRK2-NNWR algorithm for the coupling of different materials. $\Delta x = 1/50$, $[T_0, T_f] = [0, 1]$, $TOL = 1e-11, 1e-10, .., 1e-4$.

Finally, we have also included a comparison between the multirate SDIRK2-NNWR algorithm in [13] and the time adaptive SDIRK2-NNWR algorithm introduced in this paper. Figure 2 shows the global error as a function of work for the multirate and the time adaptive methods. Specifically, to compute the work we have added together all the timesteps performed on both subdomains over all the iterations. The stepsizes Δt_m, $m = 1,2$ for the multirate case are chosen to be the minimum stepsizes of the time adaptive case on each subdomain. In order to get the relation between the number of timesteps and the global error, we measure those for a decreasing sequence of tolerances starting with $TOL = 1e-1$ and ending with $TOL = 1e-6$. One observes in figure 2 how the time adaptive scheme gives a way more accurate solution than the multirate scheme employing less work. This difference increases when tolerance decreases.



(a) *Air-steel* (b) *Air-water*

Fig. 2 Comparison between time adaptive and multirate SDIRK2-NNWR algorithm. Global error as a function of work with respect to the total number of timesteps for the coupling of different materials. $\Delta x = 1/50$, $[T_0, T_f] = [0, 1]$ and $TOL = 1e-6, 1e-5, .., 1e-1$.

In conclusion, the numerical results just presented show that the time adaptive SDIRK2-NNWR algorithm introduced in this chapter is a more efficient method for the one-dimensional coupling of different combinations of materials than the multirate SDIRK2-NNWR algorithm in [13].

7 Conclusions and Further Work

We have introduced a time adaptive version of the multirate SDIRK2-NNWR method in [13]. We inserted two different controllers in the Dirichlet solvers to build two independent time grids τ_1 and τ_2 increasing the efficiency of the algorithm. The numerical results show the advantages of the time adaptive method over the previous multirate approach [13]. Unfortunately, preliminary results for the 2D extension

of the time adaptive SDIRK2-NNWR algorithm give a convergent scheme but its performance is not as good as in 1D.

Many aspects of the time adaptive approach are left for further research. The extension of the approach to higher dimensions, investigate alternatives adding time step controllers on the Neumann problems as well, implement time adaptivity with respect to macrosteps or study the influence of the initial condition on the performance of the method. Another future direction would be to use the time adaptive multirate approach explained in this paper to simulate nonlinear thermal FSI test cases.

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