Towards 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 [12]. Some work has already been done regarding time adaptive multirate methods for the simulation of FSI problems. A time adaptive partitioned approach based on the Dirichlet-Neumann iteration for thermal FSI was presented in [4, 5]. However, the Neumann-Neumann method is inherently parallel. In [10], 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 [9, 8, 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

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of different spatial and time discretizations for each subdomain. In [13], 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 article [12], we proposed and analyzed a parallel multirate partitioned approach based on the NNWR algorithm [9, 8, 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 [9, 8]. 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:

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

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:

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

Finally, the interface values are updated with

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

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, 12].

In [12, 11], 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). By making use of properties of Toeplitz matrices, we found the optimal relaxation parameter Θ_{opt} in 1D assuming implicit Euler in time, structured spatial grids and conforming time grids on both subdomains. Θ_{opt} then depends on the material coefficients α_1, α_2,

λ_1, λ_2, the spatial resolution Δx and the time resolution Δt. In the limits of $\Delta t/\Delta x^2$ to zero and to infinity, respectively, the optimal relaxation parameter is given by

$$\Theta^0_{opt} = \frac{\alpha_1\alpha_2}{(\alpha_1+\alpha_2)^2}, \quad \Theta^\infty_{opt} = \frac{\lambda_1\lambda_2}{(\lambda_1+\lambda_2)^2}. \tag{6}$$

Using Θ_{opt}, we get the exact solution at the interface after one iteration, leaving only to solve the two Dirichlet problems once. We then showed numerically that the nonmultirate 1D Θ_{opt} gives excellent estimates for the multirate case using SDIRK2 both in 1D and 2D.

4 Time adaptive method

We now introduce a new adaptive scheme that, in contrast to the multirate method in [12], increases efficiency by allowing larger step sizes without increasing the error of the numerical solution. We build our partitioned time adaptive approach on the SDIRK2-NNWR algorithm introduced in [11, chap. 6] and in [12]. 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 [7, chap. IV.8].

In our approach, time adaptive integrators for 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

$$\mathbf{r}_m^{n+1} = \mathbf{u}_I^{(m),n+1} - \hat{\mathbf{u}}_I^{(m),n+1}, \tag{7}$$

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) for implicit Runge-Kutta methods of order p introduced by [14, 15],

$$\Delta t_m^{n+1} = \Delta t_m^n \left(\frac{tol}{\|\mathbf{r}_m^{n+1}\|_2}\right)^{1/6p} \left(\frac{tol}{\|\mathbf{r}_m^{n}\|_2}\right)^{1/6p}, \tag{8}$$

on the subdomain Ω_m for $m = 1, 2$ respectively and $p = 2$ for SDIRK2. In the first step, the estimate of the previous local error $\mathbf{r}_m^0$ is not available and then we use $\mathbf{r}_m^0 = tol$.

In order to start the integration, one also needs to pick an initial step size. We use the following formula suggested by Gustaf Söderlind and inspired by [1, pp. 682-683] which is dependent on the rhs of the ODE evaluated at t_0, i.e, $f(\mathbf{u}_0)$:

$$\Delta t_m^0 = \frac{|T_f - T_0| \cdot tol^{1/2}}{100 \cdot (1 + \|f(\mathbf{u}_0)\|_2)} = \frac{|T_f - T_0| \cdot tol^{1/2}}{100 \cdot \left(1 + \|\mathbf{M}_{II}^{(m)^{-1}} \mathbf{A}_{II}^{(m)} \mathbf{u}_I^{(m),0}\|_2\right)}, \tag{9}$$

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 of the first equation in (3) respectively.

We choose the inner time adaptive tolerance finer than the outer tolerance TOL used to terminate the iteration. Specifically, we take $tol = TOL/5$ for $m = 1, 2$. This choice is motivated by [16] and already used in a similar context in [3, sec. 6].

4.1 Relaxation parameter in the time adaptive case

The aim here is to adapt the formula derived for Θ_{opt} for a fixed step size Δt in [12] to the variable step size context. We propose to start the algorithm with an initial guess for Θ and update the value after each iteration once the time grids τ_1 and τ_2 have already been computed.

For the non adaptive SDIRK2-NNWR, it was observed in [12] that the optimal relaxation parameter moves between the spatial and the temporal limits (6) of Θ_{opt} in terms of $\Delta t/\Delta x^2$. Therefore, we suggest to take an intermediate value between the two limits for the first iteration. 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.

To update the relaxation parameter after each iteration, we average all 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 by inserting the the larger of the averaged time steps into the formula from [12] for the fixed time step multirate SDIRK2-NNWR algorithm.

5 Numerical results

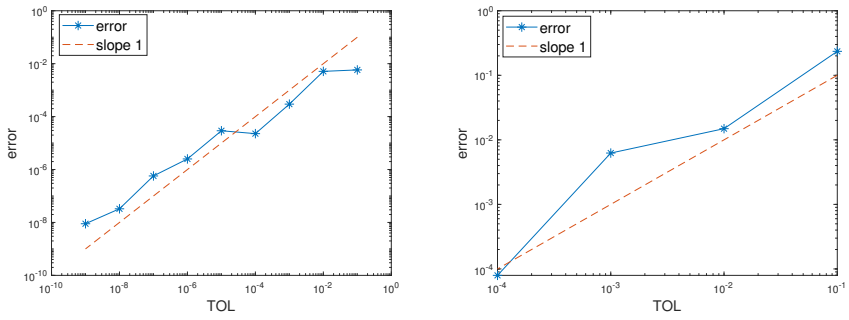
All the results in this section have been produced by implementing the algorithm in Python using the classical 1D or 2D linear FE discretization on equidistant and identical triangular meshes on both subdomains and using as a initial condition the smooth function $g(x) = -1668x^4 + 5652x^3 - 5553x^2 + 1842x$ in 1D or $g(x, y) = 2\sin(\pi y^2)\sin((\pi x^2)/2)$ in 2D on the domain $\Omega = \Omega_1 \cup \Omega_2 = [0, 1] \cup [1, 2]$ or $\Omega = \Omega_1 \cup \Omega_2 = [0, 1] \times [0, 1] \cup [1, 2] \times [0, 1]$ respectively. Physical properties of the materials are shown in table 1.

Figure 1 shows the global error of the overall solution on Ω with respect to the tolerance for the coupling between air and steel in 1D and 2D. They have been

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

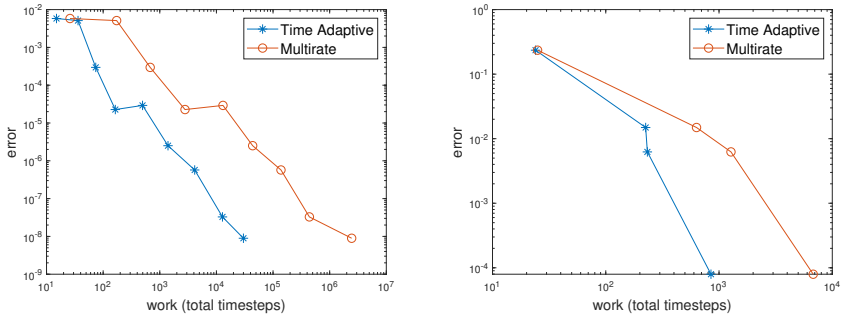
calculated with respect to a reference solution u_{ref} that has been computed using the time adaptive SDIRK2-NNWR algorithm for a very fine tolerance. One observes in Figure 1 how the error decreases proportionally to the tolerance as expected in a time adaptive numerical method.



(a) Air-water 1D **(b)** Air-steel 2D

Fig. 1: Global error as a function of the tolerance of the time adaptive SDIRK2-NNWR algorithm for different couplings in 1D and 2D. Figure (a): $\Delta x = 1/50$, $[T_0, T_f\,] = [0, 1]$ and $TOL = 1e-9, 1e{-}8, .., 1e{-}1$. Figure (b): $\Delta x = 1/10$, $[T_0, T_f\,] = [0, 100]$ and $TOL = 1e{-}4, 1e{-}3, .., 1e{-}1$.

Finally, we compare the performance of the multirate SDIRK2-NNWR algorithm with fixed time steps in [12] to the time adaptive SDIRK2-NNWR algorithm introduced in this paper. Figure 2 shows the global error as a function of work for both variants. To compute the work we added together all timesteps performed on both subdomains over all iterations. The stepsizes $\Delta t_m, m = 1, 2$ for the multirate case are the minimum stepsizes chosen by the time adaptive algorithm on each subdomain. This way, the methods produce almost the same error. In order to get the relation between the number of timesteps and the global error, we measure both magnitudes for a decreasing sequence of tolerances. Number of iterations are specified in table 2. Figure 2 shows that the time adaptive curve is below the multirate curve meaning that less work is employed to reach the same accuracy of the solution using the time adaptive scheme. This difference increases when the tolerance decreases. In 1D this results in 100 times less time steps and in the more relevant 2D case, in 10 times less time steps.



(a) Air-water 1D **(b)** Air-steel 2D

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 different couplings in 1D and 2D. Figure (a): $\Delta x = 1/50$, $[T_0, T_f\,] = [0, 1]$ and $TOL = 1e-9, 1e-8, .., 1e-1$. Figure (b): $\Delta x = 1/10$, $[T_0, T_f\,] = [0, 100]$ and $TOL = 1e-4, 1e-3, .., 1e-1$.

Table 2: Total number of fixed point iterations (FPI) and total number of timesteps over all FPI (Work) of the time adaptive SDIRK2-NNWR algorithm for different tolerances.

TOL	$1e-1$	$1e-2$	$1e-3$	$1e-4$	$1e-5$	$1e-6$	$1e-7$	$1e-8$	$1e-9$
FPI 1D	4	6	8	10	14	15	15	15	11
FPI 2D	3	15	10	16	19	-	-	-	-
Work 1D	15	36	74	164	496	1397	4135	12796	29996
Work 2D	24	225	233	849	1023	-	-	-	-

However, the method is not as robust in 2D as in 1D and fails for tolerances smaller than $1e-5$. This is because the convergence rate is extremely sensitive to the relaxation parameter. Due to lack of better choices, we use the optimal parameter from 1D in 2D, and combined with the adaptive time step this apparently leads to decreased robustness.

6 Conclusions and Further Work

We have introduced a time adaptive extension of the multirate SDIRK2-NNWR method in [12]. 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 new algorithm achieves the same solution as the multirate SDIRK2-NNWR algorithm in [12] while optimizing the number of time steps. Numerical results show that the time adaptive method uses 100 times less time steps than the multirate

method in 1D and 10 times less time steps in 2D. However, the 2D extension of the time adaptive SDIRK2-NNWR algorithm is not as robust as the 1D version.

Many aspects of the time adaptive approach are left for further research. The extension of the approach to 3D, 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 apply the time adaptive multirate approach explained in this paper to nonlinear thermal FSI cases.

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