Parareal Schwarz Waveform Relaxation Methods

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This work was in part supported by the International Science and Technology Cooperation Program of China under grant 2010DFA14700.

1 Introduction

Solving an evolution problem in parallel is naturally undertaken by trying to parallelize the algorithm in space, and then still follow a time stepping method from the initial time $t = 0$ to the final time $t = T$. This is especially easy to do when an explicit time stepping method is used, because in that case the time step for each component is only based on past, known data, and the time stepping can be performed in an embarrassingly parallel way. If one uses implicit time stepping however, one obtains a large system of coupled equations, and thus the linear or non-linear solver needs to be parallelized, e.g. using a domain decomposition method.

Over the last decades, people have however also tried to parallelize algorithms in the time direction. One example is Womble's algorithm [22], where the systems arising from an implicit time discretization are solved using an iterative method, and the iteration of the next time level is started, before the iteration on the current time level has converged. It is then possible to iterate several time levels simultaneously, but the possible gain using a parallel computer is only small, see for example [3].

A different approach to obtain small scale parallelism in time is to use predictor-corrector methods, where the prediction step and the correction step can be performed by two (or several) processors in parallel, if organized properly. An entire class of such methods has been proposed in [19], and good small scale parallelism can be achieved.

A third, very different approach are the waveform relaxation algorithms, invented in [15], which are based on a decomposition of the system to be solved into subsystems. An iteration is then used, which solves time dependent problems in each subsystem and communicates information at interfaces to neighboring subsystems to converge to the overall solution in space-time [12, 13]. Substantial progress has been made on such methods for evolution PDEs, see for example [5, 6, 14], and references

R. Bank et al. (eds.), *Domain Decomposition Methods in Science and Engineering XX*, Lecture Notes in Computational Science and Engineering 91,
DOI 10.1007/978-3-642-35275-1__53,

therein. If a multi-grid decomposition is used, instead of a domain decomposition, one obtains the so called parabolic multi-grid methods [11], which are also called multi-grid waveform relaxation methods. For further results, see [17, 21].

Finally, the last class of methods, which focuses entirely on the parallelization in the time direction, are based on shooting methods in time. A first historical step in this direction is [20], and for an early analysis see [2]. The newest algorithm in this class is the parareal algorithm, invented in [16]. For a complete historical overview of such methods, further references, and a precise convergence estimate of the parareal algorithm see [4, 9].

We propose here a space time parallel algorithm for solving evolution partial differential equations, and use as a model problem

$$\begin{aligned} \partial_t u &= \partial_{xx} u \quad \text{in } \Omega = (0,1) \times (0,T), \\ \mathscr{B}^- u(0,t) &= g_0(t) \ \ t \in (0,T), \\ \mathscr{B}^+ u(1,t) &= g_1(t) \ \ t \in (0,T), \\ u(x,0) &= u_0(x) \ \ x \in \Omega. \end{aligned} \tag{1}$$

Here $\mathscr{B}^{\pm}$ represent some boundary operators, like the identity for a Dirichlet condition, or a normal derivative for a Neumann condition. The algorithm is based on a decomposition of the space-time domain into space-time subdomains, as indicated in Fig. 1. In order to solve an evolution problem by only solving problems in small space-time domains, one has to iteratively calculate more and more accurate initial and boundary conditions for each space-time subdomain. The parareal Schwarz waveform relaxation algorithm does this by using a parareal approximation for the initial conditions, and a Schwarz waveform relaxation algorithm for the boundary conditions. For a different variant of combining a spatial and a time decomposition, see [18].

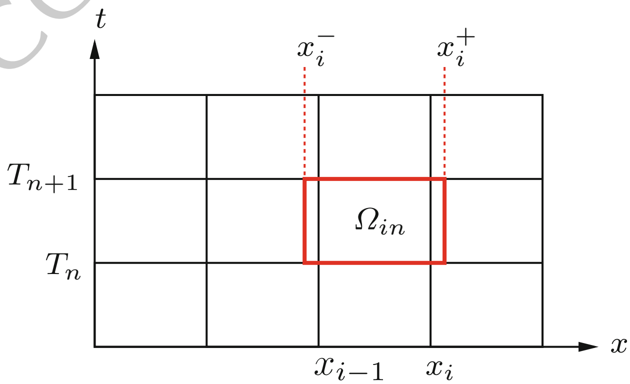

Fig. 1. Space time decomposition for the parareal Schwarz waveform relaxation algorithm

2 Parareal Schwarz Waveform Relaxation Algorithms

The parareal algorithm for the model problem (1) is based on a decomposition of the time interval $(0,T)$ into subintervals, given by $0 = T_0 < T_1 < T_2 < \ldots < T_N = T$, and the algorithm is defined using two propagation operators: a coarse operator $G(t_2,t_1,u_1,g_0,g_1)$ which provides a rough approximation of the solution $u(x,t_2)$ of (1) with a given initial condition $u(x,t_1) = u_1(x)$ and boundary conditions g_0 and g_1, and a fine operator $F(t_2,t_1,u_1,g_0,g_1)$, which gives a more accurate approximation of the same solution with initial condition $u(x,t_1) = u_1(x)$ and boundary conditions g_0 and g_1. Starting with a first approximation U_n^0 at the time points $T_0,T_1,T_2,\ldots,T_{N-1}$, the parareal algorithm performs for $k = 0,1,2,\ldots$ the correction iteration

$$U_{n+1}^{k+1} = F(T_{n+1},T_n,U_n^k,g_0,g_1) + G(T_{n+1},T_n,U_n^{k+1},g_0,g_1) - G(T_{n+1},T_n,U_n^k,g_0,g_1), \tag{2}$$

which is nothing else than a multiple shooting method with an approximate Jacobian in the Newton step, see for example [9], which also contains a precise convergence estimate for the case of the heat equation, or [4] for a similar precise convergence estimate for the case of nonlinear problems.

In contrast to the parareal algorithm, a Schwarz waveform relaxation method for the model problem (1) is based on a spatial decomposition only, in the most general case into overlapping subdomains $\Omega = \cup_{i=1}^{I}(x_i^-,x_i^+)$, as shown in Fig. 1. Here the boundaries $x_i^\pm$ of the overlapping subdomains are constructed from a non-overlapping decomposition given by the decomposition $0 =: x_0 < x_1 < \ldots < x_I := 1$, by adding and subtracting half the overlap, $x_i^- := x_{i-1} - \frac{L}{2}$, $x_i^+ := x_i + \frac{L}{2}$, except for the first and last point, $x_1^- = x_0$ and $x_I^+ = x_I$. Given an initial guess at the interfaces, say $\mathscr{B}_i^\pm u_i^0$, the Schwarz waveform relaxation algorithm solves iteratively for $k = 1,2,\ldots$ the subdomain problems

$$\begin{aligned}
\partial_t u_i^k &= \partial_{xx} u_i^k && \text{in } \Omega_i \times (0,T),\\
u_i^k(x,0) &= u_0 && \text{in } \Omega_i,\\
\mathscr{B}_i^- u_i^k(x_i^-,t) &= \mathscr{B}_i^- u_{i-1}^{k-1}(x_i^-,t) && t \in (0,T),\\
\mathscr{B}_i^+ u_i^k(x_i^+,t) &= \mathscr{B}_i^+ u_{i+1}^{k-1}(x_i^+,t) && t \in (0,T).
\end{aligned} \tag{3}$$

Here again, the operators $\mathscr{B}_i^\pm$ are transmission operators: in the case of the identity, we have the classical Schwarz waveform relaxation algorithm; for Robin or higher order transmission conditions, one would obtain an optimized Schwarz waveform relaxation algorithm, if the parameters in the transmission conditions are chosen to optimize the convergence of the algorithm, see [1, 5].

Parareal Schwarz waveform relaxation algorithms combine the two techniques for a general space-time decomposition given in Fig. 1. We propose among the many possibilities the following one: given initial conditions $u_{0,i,n}^k(x)$ and boundary conditions $\mathscr{B}_i^- u_{i-1,n}^k(t)$ and $\mathscr{B}_i^+ u_{i+1,n}^k(t)$ for $i = 1,2,\ldots,I$ and $n = 1,2,\ldots,N$ we compute

1. All accurate approximations $u_{i,n}^{k+1}(x,t) := F_{i,n}(u_{0,i,n}^k, \mathscr{B}_i^- u_{i-1,n}^k, \mathscr{B}_i^+ u_{i+1,n}^k)$ in parallel using the more accurate evolution operator.

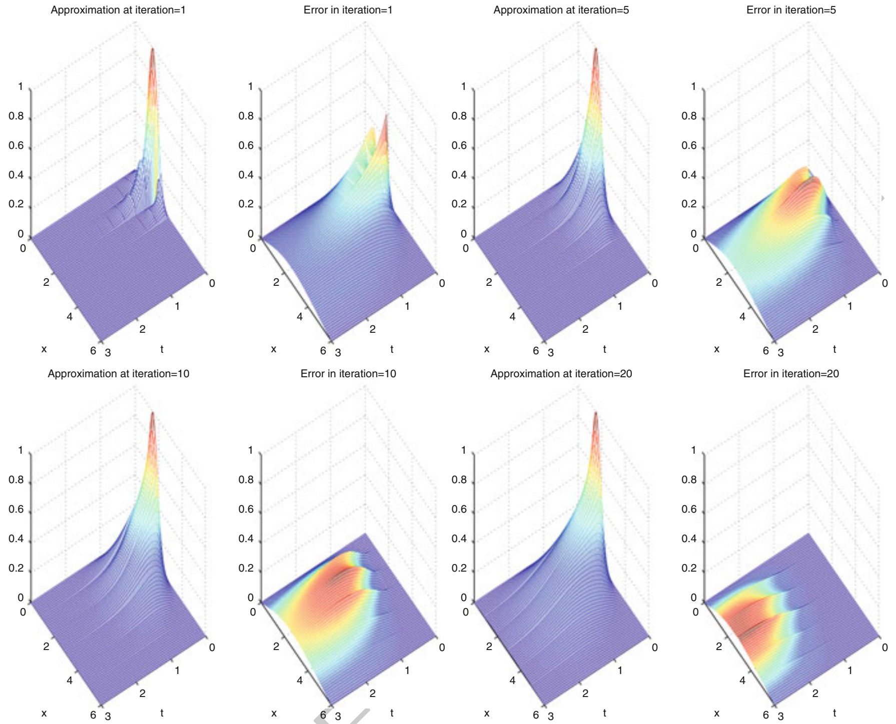

Fig. 2. Illustration how the parareal Schwarz waveform relaxation algorithm removes the error over several iterations: each plot pair shows on the *left* the approximation and on the *right* the error (i.e. the difference between the monodomain solution and the current iterate) for $k = 1, 5, 10, 20$

2. For $n = 0, 1, \ldots$, new initial conditions using a parareal integration step both in space and time,

$$u^{k+1}_{0,i,n+1} = u^{k+1}_{i,n}(\cdot, T_{n+1}) + G_{i,n}(u^{k+1}_{0,i,n}, \mathscr{B}^-_i u^{k+1}_{i-1,n}, \mathscr{B}^+_i u^{k+1}_{i+1,n})$$
$$-G_{i,n}(u^k_{0,i,n}, \mathscr{B}^-_i u^k_{i-1,n}, \mathscr{B}^+_i u^k_{i+1,n}).$$

An example on how this algorithm converges is given in Fig. 2.

We present now a first convergence result for the parareal Schwarz waveform relaxation algorithm:

Theorem 1 (Superlinear Convergence). *Let $F_{i,n}$ be the exact solution, $G_{i,n}$ be a backward Euler approximation in time, and the exact solution in space, and assume a decomposition of the spatial domain into two overlapping subdomains. If the algorithms uses Dirichlet transmission conditions, i.e. $\mathscr{B}^{\pm}_i = I$, the identity, then it converges superlinearly to the solution of the underlying problem.*

The proof of this theorem is too long and technical for this short paper, and will appear in [7]. We present however a detailed numerical study of how the algorithm depends on the various parameters in the following section.

3 Numerical Results

In all our experiments, except otherwise mentioned, we use the domain $\Omega = (0,6)$ and the time interval $(0,T)$ with $T = 3$, and discretize the heat equation with a centered finite difference discretization in space with $\Delta x = \frac{1}{10}$, and a backward Euler discretization in time, with $\Delta t = \frac{3}{100}$, and we use a decomposition into 6 equal spatial subdomains with overlap $2\Delta x$.

We start with the dependence on the number of time subintervals. In Fig. 3 on the left, we show the convergence of the algorithm when 1 (classical Schwarz waveform relaxation), 2, 4 and 10 time subintervals are used. This shows that the algorithm is quite insensitive to the number of time subintervals used. We also observe the typical superlinear convergence behavior of all waveform relaxation algorithms, see for example [8].

We next investigate how the convergence depends on the total time interval length T. For this experiment, leaving all other parameters the same, we choose $T \in \{0.1, 0.2, 0.4, 0.8, 1.6, 3.2\}, \Delta t = \frac{T}{100}$, and ten time subintervals for each simulation. The results are shown in Fig. 3 on the right. We clearly see that convergence is much faster on short time intervals, compared to long time intervals.

In order to test the dependence on the number of spatial subdomains, we use again all parameters as before, but now decompose the domain into 2, 3, 6 and 12 spatial subdomains, and again 10 time subintervals. We see in Fig. 4 on the left that using more spatial subdomains makes the algorithm converge more slowly. This can however be remedied by using smaller global time intervals, as for the Schwarz waveform relaxation algorithm, see [10].

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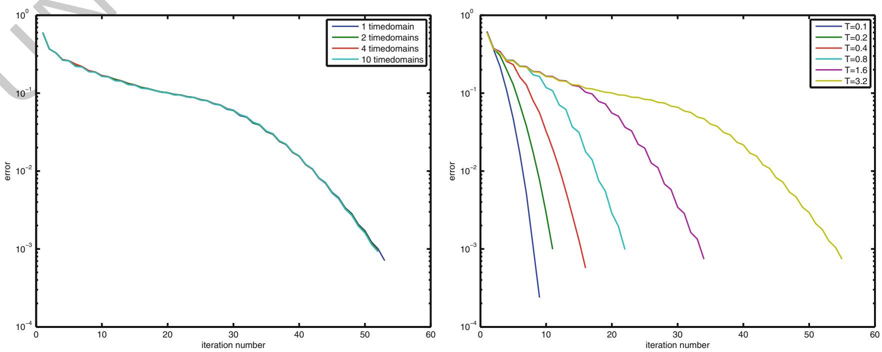

Fig. 3. Dependence of the parareal Schwarz waveform relaxation algorithm on the number of time subintervals on the *left*, and the total time window length on the *right*

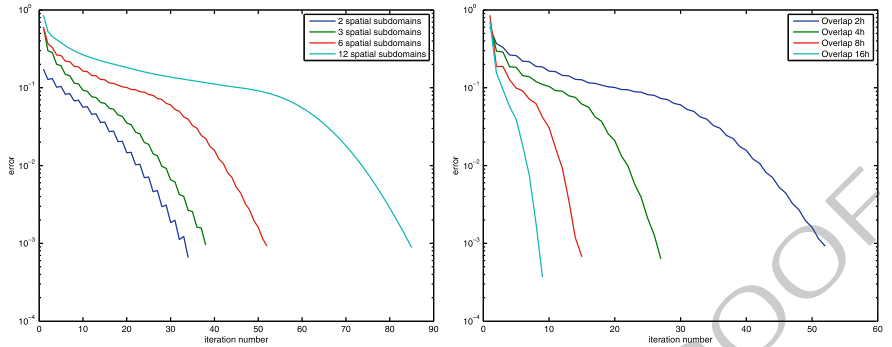

Fig. 4. Dependence of the parareal Schwarz waveform relaxation algorithm on the number of spatial subdomains on the *left*, and the overlap on the *right*

We finally test the dependence on the overlap, using $2\Delta x$, $4\Delta x$, $8\Delta x$ and $16\Delta x$ for the overlap. We see on the right in Fig. 4 that increasing the overlap substantially improves the convergence speed of the algorithm. This increases however also the cost of the method, since bigger subdomain problems need to be solved.

A better approach is to use optimized transmission conditions, see for example [1, 5]. Using the same configuration as in the previous experiment, and $2\Delta x$ overlap, we obtain with first order transmission conditions and choosing the parameters $p = 1$, $q = 1.75$ (for terminology, see [1]) the result shown in Fig. 5. This illustrates well that using optimized transmission conditions can lead to even better performance of the algorithm than very generous overlap, at no additional cost, since the subdomain size and matrix sparsity is the same as for the case of Dirichlet transmission conditions. In addition we observe that now the convergence has become more linear, and the

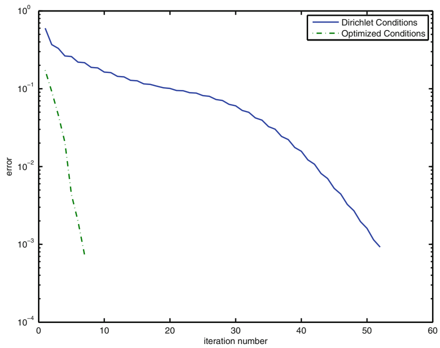

Fig. 5. Comparison of the parareal Schwarz waveform relaxation algorithm with Dirichlet and optimized transmission conditions

algorithm does not depend significantly any more on the superlinear convergence mechanism essential with Dirichlet transmission conditions.

4 Conclusion

We presented a general parareal Schwarz waveform relaxation algorithm, which is based on a decomposition in space and time of a given evolution problem, in order to increase parallelism. We stated a theoretical convergence result, whose proof will appear elsewhere, and then illustrated the dependence of the algorithm on the space-time decomposition configuration, which revealed that for fast convergence, either short time intervals, large overlap, or optimized transmission conditions need to be used. We are currently working on precise convergence factor estimates, a variant of the algorithm which also uses a coarse spatial mesh, and the addition of a coarse propagation mechanism over many spatial subdomains.

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