Analysis of a Modified Parareal Algorithm for Second-Order Ordinary Differential Equations

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Abstract. The parareal algorithm is a numerical method to integrate evolution problems on parallel computers. While this algorithm is effective for diffusive problems, its convergence properties are much less favorable for hyperbolic problems. We analyze in this paper a recently proposed variant of the parareal algorithm for hyperbolic problems for the case of systems of second order ordinary differential equations.

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INTRODUCTION

The parareal algorithm is a time parallel time integration method for evolution problems introduced by Lions, Maday and Turinici in [1]. It can be used to compute in parallel an approximate solution of the system of ordinary differential equations (ODEs)

$$u'(t) = f(u(t)), \quad t \in (0,T), \quad u(0) = u_0, \tag{1}$$

where $f : \mathbf{R}^M \to \mathbf{R}^M$ and $u : \mathbf{R} \to \mathbf{R}^M$. First, the time domain $(0,T)$ is decomposed into N-time subdomains $\Omega_n = (T_{n-1}, T_n)$, $n = 1,2,\ldots,N$, and we set for simplicity $T_n - T_{n-1} = \Delta T$. Then, using a coarse propagator $G(T_n, T_{n-1}, v)$, which gives a rough approximation of the solution $u(T_n)$ of (1) with initial conditions $u(T_{n-1}) = v$, and a fine propagator $F(T_n, T_{n-1}, v)$, which gives a more accurate approximation, the algorithm starts with an initial approximation U_n^0, $n = 0,\ldots,N$, obtained for example from the coarse propagator,

$$U_n^0 = G(T_n, T_{n-1}, U_{n-1}^0), \quad U_0^0 = u_0, \tag{2}$$

and then performs for $k = 0,1,\ldots$ the correction iteration

$$U_{n+1}^{k+1} = G(T_{n+1}, T_n, U_n^{k+1}) + F(T_{n+1}, T_n, U_n^k) - G(T_{n+1}, T_n, U_n^k). \tag{3}$$

Gander and Vandewalle showed in [2] that the parareal algorithm is a multiple shooting method for initial value problems with a coarse grid approximation for the Jacobian in Newtons method. They also showed that when the method is applied to linear, diffusive problems, it converges linearly on long time intervals and superlinearly on short time intervals. Gander and Hairer showed in [3] the following general convergence result for the non-linear case:

Theorem 1 *If the coarse propagator G is a numerical method of order p satisfying*

$$|G(t+\Delta T, t, v) - G(t+\Delta T, t, w)| \le (1 + C\Delta T)|v - w|, \tag{4}$$

the fine propagator F is exact, and their difference can be expanded for ΔT small,

$$F(T_n, T_{n-1}, v) - G(T_n, T_{n-1}, v) = c_{p+1}(v)\Delta T^{p+1} + c_{p+2}(v)\Delta T^{p+2} + \ldots, \tag{5}$$

then the error at step k of the parareal algorithm (3) satisfies the convergence estimate

$$|u(T_n) - U_n^k| \le C_1 \frac{(C_2 T_n)^{k+1}}{(k+1)!} e^{C(T_n - T_{k+1})} \Delta T^{p(k+1)}. \tag{6}$$

In [3], [4], [5], the authors showed that the parareal algorithm produces a speed-up for first order ODEs, but the method does not have the same potential for second order ODEs, see also [2].

THE MODIFIED PARAREAL ALGORITHM

We are interested in solving in parallel systems of second order ODEs of the form

$$Mq'' + Dq' + Kq = f(t), \quad q(t_0) = q_0, \quad q'(t_0) = q'_0, \tag{7}$$

where $M, D, K \in \mathbf{R}^{N' \times N'}$ represent the mass, the damping and the stiffness matrices. We first consider the homogeneous case, and rewrite (7) as a first order system,

$$u' = Au, \, u(t_0) = u_0, \tag{8}$$

to which the parareal algorithm (3) can now be applied. The inefficiency of this algorithm for second order ODEs is caused by a beating phenomenon, as explained in [6], due to the use of the coarse propagator G in (3) when computing $G(T_{n+1}, T_n, U_n^{k+1} - U_n^k)$ in this linear case. Farhat and collaborators proposed in [6] to use the fine propagator F for the part of $U_n^{k+1} - U_n^k$ in the subspace for which the evolution is already known from previous evaluations of the fine propagator F, and to only propagate the rest with the coarse propagator. Defining

$$\mathscr{S}_k = \text{span}\{U_n^l\}, \quad 0 \le l \le k, \quad 0 \le n \le N,$$

and replacing $G(T_{n+1}, T_n, U_n^{k+1} - U_n^k)$ in (3) by $K(T_{n+1}, T_n, U_n^{k+1} - U_n^k)$ defined by

$$K(T_{n+1}, T_n, V) = F(T_{n+1}, T_n, P_k V) + G(T_{n+1}, T_n, (I - P_k)V), \tag{9}$$

where P_k is the orthogonal projection into the space $\mathscr{S}_k$, we obtain the modified parareal algorithm

$$U_{n+1}^{k+1} = F(T_{n+1}, T_n, P_k U_n^{k+1}) + G(T_{n+1}, T_n, (I - P_k)U_n^{k+1}), \tag{10}$$

where we used linearity again, and the fact that $P_k U_n^k = U_n^k$ and $(I - P_k)U_n^k = 0$. To obtain the next approximation at step $k+1$ of this new algorithm, one first has to compute $F(T_{n+1}, T_n, U_n^k)$ in parallel for all n, to know the fine evolution of the initial conditions U_n^k of the current step. Now that their evolution is known, the space $\mathscr{S}_k$ can be extended by adding these initial conditions,

$$\mathscr{S}_k = \mathscr{S}_{k-1} \cup \text{span}\{U_n^k\}, \qquad \mathscr{S}_0 = \text{span}\{U_n^0\},$$

and a basis of $\mathscr{S}_k$ is computed using the QR-factorization. Let S_k be the matrix formed by the orthogonal basis column vectors of $\mathscr{S}_k$. The projection P_k is then defined by

$$P_k = S_k (S_k^T Q S_k)^{-1} S_k^T Q, \qquad Q = \begin{pmatrix} \mathrm{M} & 0 \\ 0 & \mathrm{K} \end{pmatrix}. \tag{11}$$

Now the cheap sequential step in (10) over index n is performed, starting with $U_0^{k+1} = U_0^0$, by calculating for each n the projection $P_k U_n^{k+1}$, for which the fine evolution is known and no extra computation is necessary, and the remaining part $(I - P_k)U_n^{k+1}$ is then propagated using the coarse propagator G.

Note that in the linear case, the space $\mathscr{S}_k$ can be interpreted as a Krylov space for the linear propagator F with multiple right hand sides corresponding to the number of time intervals of the method.

CONVERGENCE ANALYSIS

We assume that the initial condition of the problem is a linear combination of eigenmodes of the linear operator A, $A\phi_j = \lambda_j \phi_j$, and excites l of those natural modes, $U_0 = \alpha_1 \phi_1 + \ldots + \alpha_l \phi_l$. Our first result shows that the new parareal algorithm converges in a finite number of steps, and is very much related to the convergence behavior of Krylov methods.

Theorem 2 *The new parareal algorithm (10) converges as soon as $\mathscr{S}_{k-1} = \mathscr{S}_k$. Furthermore, we have that $\mathscr{S}_n \subset$ span$\{\phi_1, \ldots, \phi_l\}$ for all n.*

Our second convergence result for the modified parareal algorithm includes the use of an approximate fine propagator. We denote by $\tilde{F}$ the exact solution of the equation, and we assume that the difference between the exact solution and the coarse approximation obtained from G can be expanded for ΔT small,

$$\tilde{F}(T_n,T_{n-1},v) - G(T_n,T_{n-1},v) = c_{p+1}(v)\Delta T^{p+1} + c_{p+2}(v)\Delta T^{p+2} + \dots. \tag{12}$$

The fine propagator F is now a numerical method defined on each time subdomain Ω_n. For simplicity, we assume that each Ω_n is discretized by the same time step of size $\Delta t = \Delta T/M$, and thus on the fine mesh we have $\Delta t = t_m - t_{m-1}$, $m = 1,2,\dots M$. We furthermore also assume that the difference of the exact solution $\tilde{F}$ and the fine propagator F can be expanded for Δt small,

$$\tilde{F}(t_m,t_{m-1},v) - F(t_m,t_{m-1},v) = c'_{p+1}(v)\Delta t^{p+1} + c'_{p+2}(v)\Delta t^{p+2} + \dots. \tag{13}$$

We also assume that both the coarse propagator G and the fine propagator F satisfy the Lipschitz condition (4). We can then prove the following result:

Theorem 3 *Let $|\cdot|$ be the norm on $\mathbf{R}^N$ associated with the metric given by the matrix Q (the metric of the projector P_k). If the propagators F and G are of order p, then the hybrid propagator K is also of order p, and satisfies*

$$|\tilde{F}(T_{n+1},T_n,v) - K(T_{n+1},T_n,v)| \le C(\Delta t^{p+1} + \Delta T^{p+1})|v|. \tag{14}$$

Our second convergence result gives an estimate on the convergence rate of the new algorithm.

Theorem 4 *If F and G are two propagators of order p, then the error of the new parareal algorithm (10) satisfies at iteration k the estimate*

$$|u(t_n) - U_n^k| \le C_1 \frac{(C_2 T_n)^{k+1}}{(k+1)!} e^{C(T_n - T_{k+1})} \Delta T^{p(k+1)} + C_3 T e^{C_4 \Delta T} \Delta t^p. \tag{15}$$

INHOMOGENEOUS CASE

We have so far only considered the homogeneous case in (8). If the problem is inhomogeneous, we can however first do a precomputation step by evaluating $F(T_{n+1},T_n,0)$ for all n, and then at each iteration we compute $F(T_{n+1},T_n,P_kU_n^{k+1})$ as follows, see [6]: let α_j^l be the coefficients of the projected vector U_n^{k+1}, $P_kU_n^{k+1} = \sum_{l,j}\alpha_j^l U_j^l$. We then evaluate

$$\begin{aligned} F(T_{n+1},T_n,P_kU_n^{k+1}) &= F(T_{n+1},T_n,\sum_{l,j}\alpha_j^l U_l^l) \\ &= \sum_{l,j}\alpha_j^l \Big(F(T_{n+1},T_n,U_j^l) - F(T_{n+1},T_n,0)\Big) + F(T_{n+1},T_n,0), \end{aligned}$$

which again does not involve any evaluation of F.

NUMERICAL EXPERIMENTS

We consider the simple model problem $u'' = -u$ with initial conditions $u(0) = 1$ and $u'(0) = 0$. We transform the equation into a system of the form (8) with two components, and perform the simulations on the time interval $[0,20]$. We choose for the coarse time step $\Delta T = 1$, and for the fine time step $\Delta t = 1/6$. In Figure 1, we show the first few iterations of the original parareal algorithm, on the left for the first component, and on the right for the second component, together with the fine grid solution. One can see that the algorithm is converging slowly, and that the convergence early in the time interval is significantly better than later in the time interval.

In Figure 2, we show the initial guess and the first iteration of the modified parareal algorithm, which converges with the first iteration. This illustrates our first convergence result, see Theorem 2, since in this low dimensional problem, the fine solution is already contained in the subspace after one iteration.

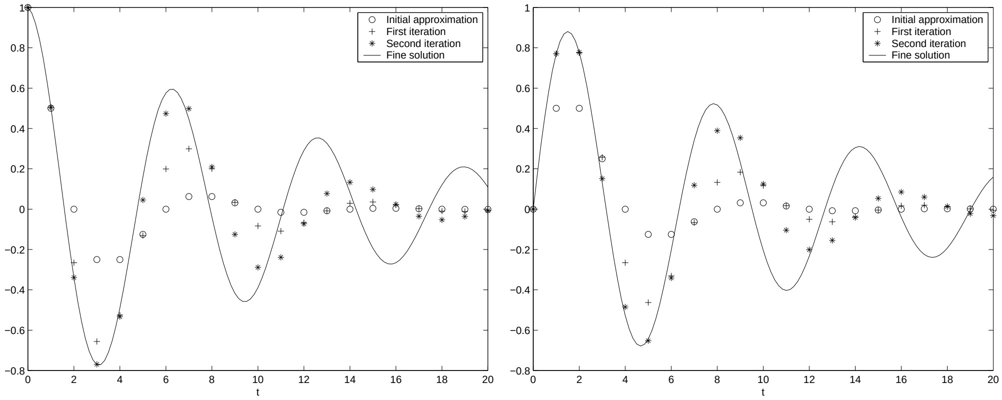

FIGURE 1. First few iterations of the original parareal algorithm for the model problem.

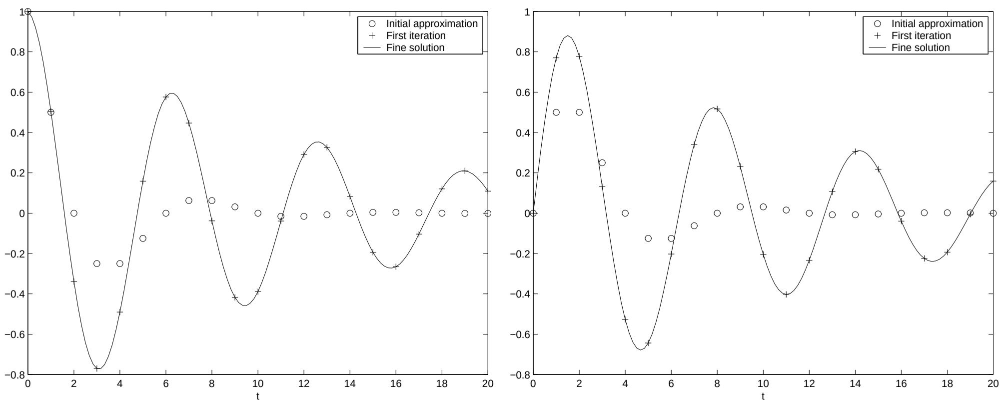

FIGURE 2. Initial approximation and first iteration of the modified parareal algorithm for the model problem.

CONCLUSIONS

We presented two new convergence results for a variant of the parareal algorithm adapted to the solution of hyperbolic problems by Farhat and collaborators [6]. The new algorithm can not only be used for hyperbolic problems, the reuse of the subspace where the evolution is known with high accuracy should be beneficial for other problems as well. It would also be of interest to find a sharper convergence estimate than the one presented in Theorem 4, using the fact that the approximation is now sought in a Krylov space, which we are currently investigating.

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