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Analysis for parareal algorithms applied to Hamiltonian differential equations

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ABSTRACT

Long-time integrations are an important issue in the numerical solution of Hamiltonian systems. They are time consuming and it is natural to consider the use of parallel architectures for reasons of efficiency. In this context the parareal algorithm has been proposed by several authors.

The present work is a theoretical study of the parareal algorithm when it is applied to Hamiltonian differential equations. The idea of backward error analysis is employed to get insight into the long-time behavior of numerical approximations. One of the main results is that convergence of the parareal iterations restricts the length of the time window. For nearly integrable systems its length is bounded by the square root of the inverse of the accuracy of the coarse integrator. The theoretical bounds are confirmed by numerical experiments.

1. Introduction

Long-time integrations of differential equations can be time consuming and it is a natural idea to consider the use of computations in parallel. In this work we restrict our attention to Hamiltonian systems of ordinary differential equations

$$\dot{y} = f(y), \qquad f(y) = J^{-1}\nabla H(y), \qquad J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}, \tag{1}$$

where the vector $y = (p, q)$ collects momenta and positions, and the smooth scalar function $H(y)$ is called Hamiltonian or energy of the system. The symbol I in the structure matrix J is the d-dimensional identity matrix, and d is the number of degrees of freedom. The exact flow $\varphi_t(y)$ is for every t a symplectic transformation, which means that its derivative with respect to the initial value satisfies

$$\varphi_t'(y)^{\mathsf{T}} J\, \varphi_t'(y) = J. \tag{2}$$

It is well known that for long-time integrations the use of symplectic methods is recommended. This means that the discrete flow $y_{n+1} = \Phi_{\Delta T}(y_n)$ should share the property (2) with the exact flow. This then implies that the energy is nearly preserved along the numerical solution; see [1].

The parareal algorithm has been introduced by Lions, Maday, and Turinici in [2] as an approach for exploiting parallel architectures in the numerical solution of real time problems. Among earlier attempts for parallel in time discretizations let

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us mention the work of Bellen and Zennaro [3], where a Steffensen-like iterative method is proposed for general difference equations, the parallel shooting technique of Chartier and Philippe [4], and the review article [5] on CWI (Amsterdam) contributions on parallel Runge–Kutta methods.

The parareal algorithm, originally proposed for the numerical treatment of partial differential equations, has also found applications in ordinary differential equations. During the last few years much research has been devoted to the long-time integration of Hamiltonian systems. The "symplectic parareal" of [6] is a non-iterative algorithm whose practical relevance has to be proven. Multi-time step parareal algorithms [7] are proposed for parallelizing in time molecular dynamics problems. The article [8] proposes a time-parallel algorithm for almost integrable Hamiltonian systems and has in mind very accurate computations in planetary motion. Our research is to a large extent motivated by [9], where symmetric parareal algorithms including projections are proposed for Hamiltonian systems.

After recalling the definition of the parareal algorithm for initial value problems of ordinary differential equations (Section 2), we present the main results, which are long-time error estimates for the parareal iterates for Hamiltonian systems, and numerical illustrations in Section 3. If ε denotes the accuracy of the coarse integrator, we show that convergence can be achieved on intervals whose length is restricted by $\mathcal{O}(\varepsilon^{-1})$ for the harmonic oscillator, by $\mathcal{O}(\varepsilon^{-1/2})$ for integrable systems, and by $\mathcal{O}(1)$ for systems with chaotic solutions. The proofs are given in Section 4 for linear problems and in Sections 5 and 6 for nonlinear problems. Section 7 shows how the analysis extends to the symmetric parareal algorithm. For high accuracy computations we present a variant of the parareal algorithm in Section 8, which permits to use quadruple precision for the fine integrator and double precision for the coarse integrator.

2. The parareal algorithm for ordinary differential equations

Consider an initial value problem of ordinary differential equations $\dot{y} = f(y), y(0) = y_0$. For a given step size ΔT we consider two discrete flow maps: a cheap approximation with low accuracy which we denote by $\varphi^G_{\Delta T}(y)$ (coarse integrator), and an accurate approximation which we denote by $\varphi^F_{\Delta T}(y)$ (fine integrator). The parareal algorithm, which is given by $u^k_0 = y_0$ for all k, and

$$\begin{aligned} u^0_{n+1} &= \varphi^G_{\Delta T}(u^0_n) \\ u^k_{n+1} &= \varphi^F_{\Delta T}(u^{k-1}_n) - \varphi^G_{\Delta T}(u^{k-1}_n) + \varphi^G_{\Delta T}(u^k_n), \end{aligned} \tag{3}$$

is expected to yield approximations that converge rapidly to the solution of the fine integrator. We use the notation

c_G cost (cpu time) of one step of the coarse integrator $\varphi^G_{\Delta T}$,
c_F cost (cpu time) of one step of the fine integrator $\varphi^F_{\Delta T}$,
K maximal number of parareal iterations,
N number of steps in one time window of length T, i.e., $N\Delta T = T$.

A *sequential computation* of the solution on an interval of length $T = N\Delta T$ with the accurate integrator $\varphi^F_{\Delta T}$ requires a total time

$$Nc_F \quad \text{with 1 processor.}$$

For the *standard application of the parareal algorithm* on the same interval one first computes sequentially the values u^0_n for all $n = 1, \dots, N$. In the kth iteration, one computes all values $\varphi^F_{\Delta T}(u^{k-1}_n)$ in parallel and subsequently the values u^k_n in a sequential manner. This requires a total time

$$Nc_G + K(Nc_G + c_F) \quad \text{with } N \text{ processors.}$$

The performance can be improved, if the different processors are able to perform different tasks at the same time. The idea is to start the computation with the integrators $\varphi^F_{\Delta T}$ and $\varphi^G_{\Delta T}$ as soon as the initial values are available. Such a procedure is called *pipelined parareal algorithm* in [10] and requires a total time $Nc_G + K(c_G + c_F)$ with N processors. A minor improvement is possible to perform the computation in a total time

$$Nc_G + Kc_F \quad \text{with } (q+1)K + 1 \text{ processors,}$$

where q denotes the smallest positive integer satisfying $c_F \le qc_G$. This can be achieved as follows: on the first processor one computes sequentially the values u^0_{n+1} for $n = 0, \dots, N-1$; in the kth iteration, q processors are used to compute $\varphi^F_{\Delta T}(u^{k-1}_n)$ for $n = k-1, \dots, N-1$, starting the computation as soon as u^{k-1}_n is available, and a further processor computes sequentially the values $\varphi^G_{\Delta T}(u^k_n)$ and u^k_{n+1} for $n = k, \dots, N-1$. The first processor requires the time Nc_G and every parareal iteration requires the additional time c_F.

In general it is not possible to treat the whole interval $[0, T_{\text{end}}]$, where the problem has to be solved, in one piece. One has to divide it into time windows on which the parareal algorithm can be applied. To get a significant benefit from the use of parallel architectures, the length T of the time window should be as large as possible. It is one of the main results of our research that this length T cannot be arbitrarily large for Hamiltonian systems and is restricted in terms of the accuracy of the coarse integrator.