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Efficient multiple time-stepping algorithms of higher order ☆

Abdullah Demirel [a], Jens Niegemann [b], Kurt Busch [c], Marlis Hochbruck [a]

[a] Institut für Angewandte und Numerische Mathematik, Karlsruher Institut für Technologie, 76128 Karlsruhe, Germany
[b] ETH Zurich, Institute of Electromagnetic Fields (IEF), 8092 Zurich, Switzerland
[c] Humboldt-Universität zu Berlin, Institut für Physik, AG Theoretische Optik & Photonik, and Max-Born-Institut, 12489 Berlin, Germany

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ABSTRACT

Multiple time-stepping (MTS) algorithms allow to efficiently integrate large systems of ordinary differential equations, where a few stiff terms restrict the timestep of an otherwise non-stiff system. In this work, we discuss a flexible class of MTS techniques, based on multistep methods. Our approach contains several popular methods as special cases and it allows for the easy construction of novel and efficient higher-order MTS schemes. In addition, we demonstrate how to adapt the stability contour of the non-stiff time-integration to the physical system at hand. This allows significantly larger timesteps when compared to previously known multistep MTS approaches. As an example, we derive novel predictor–corrector (PCMTS) schemes specifically optimized for the time-integration of damped wave equations on locally refined meshes. In a set of numerical experiments, we demonstrate the performance of our scheme on discontinuous Galerkin time-domain (DGTD) simulations of Maxwell's equations.

1. Introduction

When following a method-of-lines approach, time-dependent partial differential equations (PDEs) are typically reduced to large systems of coupled ordinary differential equations (ODEs). Often, such a system of ODEs is then integrated by an explicit ODE solver [1,2] to obtain the time evolution of the unknowns. While explicit solvers are easily implemented, this approach has the well-known problem of conditional stability. In many cases, the system contains only a few terms which force the entire simulation to take small timesteps. In the following, we assume that we can split the system of ODEs into stiff terms (which mandate a small timestep) and non-stiff terms (which permit a larger timestep) as

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{u}(t) = \mathbf{f}\big(t, \mathbf{u}(t)\big) + \mathbf{g}\big(t, \mathbf{u}(t)\big), \tag{1}$$

where $\mathbf{f}$ contains the stiff part and $\mathbf{g}$ contains the non-stiff part. In particular we assume $\mathbf{g}$ to be Lipschitz continuous.

Such split systems are very common in scientific and technical applications, where the origin of the stiffness can be vastly different. Possibly the most common reasons are

- *Algebraic stiffness*, which directly stems from large differences in the timescales of the underlying equations. Some examples are discretized convection–diffusion–reaction equations [3], molecular dynamics [4] or electrical circuits [5].

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E-mail address: marlis.hochbruck@kit.edu (M. Hochbruck).

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- *Grid-induced stiffness*, which occurs in the spatial discretization of partial differential equations (PDEs) with non-uniform meshes. Caused by small geometrical features or due to local refinement, some of the elements may require much smaller timesteps than the rest of the mesh.

A first mitigation to this problem is to employ solvers specifically designed for stiff systems, e.g., implicit solvers [6]. Unfortunately, if the number of unknowns is very large, the solution of large (and possibly nonlinear) systems of equations often is prohibitively expensive. An alternative approach towards a more efficient procedure is to treat $\mathbf{f}$ and $\mathbf{g}$ with different timesteps, i.e., carrying out many small timesteps for $\mathbf{f}$ and a few large timesteps for $\mathbf{g}$. This approach is often called multiple time-stepping (MTS) or local time-stepping (LTS). Of course, one still has to take the coupling between $\mathbf{f}$ and $\mathbf{g}$ into account which makes the construction of such techniques quite involved. Probably one of the first methods in this direction was published by Rice in 1960 [7] and started the field of multirate Runge–Kutta schemes. Similar ideas were later also applied to multistep methods [8]. Another popular approach is to employ coupled implicit (for $\mathbf{f}$) and explicit (for $\mathbf{g}$) methods, resulting in implicit-explicit (IMEX) schemes. Such schemes have been constructed for both multistep (see [9] and references therein) and Runge–Kutta methods [10]. For a brief but very recent review on general LTS techniques, also see [11]. For recent applications of LTS and IMEX schemes in the context of advection dominated problems, see [12–18].

In this paper, we present an alternative and fairly general strategy of constructing MTS methods. In contrast to most of the commonly used techniques, our approach allows to employ different time-stepping strategies for the inner (stiff) and the outer (non-stiff) integration. As an illustration, we will combine a predictor–corrector scheme for the outer integration with a low-storage Runge–Kutta method for the inner integration. This feature increases the flexibility in the design of MTS methods and, in certain cases, leads to a significant performance enhancement. Furthermore, we will show how to tailor the stability domain of the outer multistep integrator to the underlying physical problem. This can result in a significant increase in the largest stable timestep and therefore further improves the performance of our method. For certain choices of the inner integrator, our approach reduces to previously known schemes.

2. Multiple time-stepping methods

In the following, we will assume that the evaluation of the stiff function $\mathbf{f}$ is computationally cheap in comparison to the non-stiff function $\mathbf{g}$. This is usually the case for grid-induced stiffness, where a few small elements limit the stability of an otherwise large mesh.

2.1. General explicit multiple time-stepping methods

For the construction of our methods we follow an idea presented recently in [19] for semilinear problems, where $\mathbf{f}(t,\mathbf{u}(t)) = -A\mathbf{u}(t)$ with a square matrix A of possibly large dimension, i.e.,

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{u}(t) = -A\mathbf{u}(t) + \mathbf{g}\big(t,\mathbf{u}(t)\big), \quad \mathbf{u}(t_0) = \mathbf{u}_0. \tag{2}$$

A representation of the exact solution of (2) can be obtained from the variation of constants formula

$$\mathbf{u}(t_{n+1}) = e^{-hA}\mathbf{u}(t_n) + h\int_0^1 e^{-(1-\theta)hA}\mathbf{g}\big(t_n+\theta h, \mathbf{u}(t_n+\theta h)\big)\,\mathrm{d}\theta, \tag{3}$$

where $t_n := t_0 + nh$, $n \in \mathbb{N}_0$. Note that the matrix exponential e^{-tA} is uniformly bounded by one for all $t \geq 0$ if the field of values of A is contained in the right complex half plane, see, e.g., [6, Section IV.11]. An approximation to $\mathbf{u}(t_{n+1})$ can be obtained by replacing the non-stiff function $\mathbf{g}(t,\mathbf{u}(t))$ in (3) by a local interpolation polynomial as

$$\mathbf{u}(t_{n+1}) \approx \mathbf{u}_{n+1} = e^{-hA}\mathbf{u}_n + h\int_0^1 e^{-(1-\theta)hA}\mathbf{p}_n(t_n+\theta h)\,\mathrm{d}\theta \tag{4}$$

and to computing the integral in (4) exactly. The resulting methods are known as exponential multistep methods of Adams-type. They have been first discussed in [20] and in a more systematic way in [21]. A rigorous error analysis was given in [19]. As noted in [19], the approximation $\mathbf{u}_n \approx \mathbf{u}(t_n)$ of an exponential multistep method of Adams type coincides with the exact solution $\mathbf{v}_n(h)$ of the following initial value problem

$$\frac{\mathrm{d}}{\mathrm{d}\tau}\mathbf{v}_n(\tau) = -A\mathbf{v}_n(\tau) + \mathbf{p}_n(t_n+\tau), \quad \tau \in [0,h],\ \mathbf{v}_n(0) = \mathbf{u}_n. \tag{5}$$

Here, $\mathbf{p}_n(t)$ is defined as the local interpolation polynomial which approximates $\mathbf{g}(t,\mathbf{u}(t))$ on the time interval $[t_n, t_{n+1}]$. The key idea of these methods is based on the local polynomial approximation of the non-stiff function $\mathbf{g}(t,\mathbf{u}(t))$ instead of using a local polynomial approximation of the complete right-hand side, as in the classical case.