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Preconditioned implicit-exponential integrators (IMEXP) for stiff PDEs

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ABSTRACT

We propose two new classes of time integrators for stiff DEs: the implicit exponential (IMEXP) and the hybrid exponential methods. In contrast to the existing exponential schemes, the new methods offer significant computational advantages when used with preconditioners. Any preconditioner can be used with any of these new schemes. This leads to a broader applicability of exponential methods. The proof of convergence of these integrators and numerical demonstration of their efficiency are presented.

1. Introduction

Many problems in science and engineering are characterized by the presence of a wide range of spatial and temporal scales in the phenomenon under investigations. Complex interactions of numerous processes evolving on different scales can cause the differential equations describing the evolution of the system to be stiff. Solving such stiff large systems of differential equations numerically is a challenging task. In particular, in many applications large scale systems of ordinary differential equations, which often result from spatial discretization of partial differential equations, have to be solved numerically over very long time intervals compared to the fastest processes in the system. Development of an efficient time integrator that enables simulation of such systems in a reasonable time requires much effort and care since standard methods can be too computationally expensive. A custom designed time integrator which exploits the structure of the problem and the source of stiffness can bring the necessary computational savings that enable simulation of the problem in the parameter regimes of interest. In this paper we address a class of initial value problems which can be written in the form

$$u'(t) = F(u(t)) = L(u(t)) + N(u(t)), \qquad u(t_0) = u_0, \tag{1.1}$$

where both differential operators L and N can be stiff. Often L is a linear operator that represents, for instance diffusion. If N is not a stiff operator, equations of type (1.1) are usually solved using implicit–explicit (IMEX) integrators. IMEX schemes have been widely used in a variety of fields with some of the earlier applications coming from fluid dynamics in conjunction with spectral methods [1,2]. An example of one of the most widely used, particularly in the context of large-scale applications, IMEX schemes, is the second order BDF-type method (we will call it here 2-sBDF) which was proposed in [3], one of the first publications where IMEX methods were systematically analyzed and derived. Over the past decades a range of

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IMEX schemes have been introduced such as, for example, linear multistep [3,4], Runge–Kutta [5] and extrapolated [6] IMEX methods. Such schemes have proven to be very efficient for problems such as advection–diffusion equations or reaction–diffusion equations where advection or reaction are slow and diffusion is occurring on a fast time scale. Diffusion in this case is treated implicitly while advection or reaction terms are treated with an explicit method. The IMEX methods are particularly efficient if a good preconditioner is available to speed up convergence of an iterative method used in the implicit solver. Construction of an efficient preconditioner is the topic of extensive research and software development; frequently the majority of time spent on development and implementation of an IMEX scheme for a large scale problem goes to creating a preconditioner [7]. The complexity of a differential operator that has to be preconditioned is directly related to the difficulty in constructing an efficient preconditioner. For example, a large number of preconditioners have been developed for the Laplacian operator which models linear diffusion process.

While IMEX schemes work well if L is a stiff operator and N is not, in many applications both of these terms introduce stiffness. Such problems arise from a wide range of fields, from electrochemistry [8] to combustion [9] and plasma physics [10]. A reaction–diffusion system describing chemical kinetic mechanisms involved in ignition of different chemical mixtures can involve thousands of reactions occurring over a wide range of time scales comparable to those of the diffusive processes in the system [9]. Similar structure can be encountered in models of electrochemical material growth where for certain parameter regimes the reactive terms can be as stiff as the diffusive operators in the equations [8]. In magnetohydrodynamic (MHD) equations describing the large scale plasma behavior, stiffness arises from the presence of a wide range of waves encoded in the complex nonlinear terms of the system [11]. While the IMEX or closely-related semi-implicit integrators are typically used for these problems, their performance suffers. The stiffness of the nonlinear operator N which is treated explicitly imposes prohibitive stability restrictions on the time step size. Abandoning the IMEX approach in this case and using a method that treats $N(u(t))$ implicitly as well, also poses a computational challenge. The operator N can be very complex and development of an efficient preconditioner to enable implicit treatment of this term might be difficult or even impossible.

Recently exponential integrators emerged as an efficient alternative to standard time integrators for solving stiff systems of equations. It has been shown that exponential time integrators can offer significant computational savings, particularly for large scale stiff systems, in comparison to implicit Newton–Krylov methods [12–19]. However, such comparisons are valid for problems where no efficient preconditioner is available for the implicit Newton–Krylov integrators. A shortcoming of the exponential integrators is that, at present, there are no algorithms that can utilize preconditioners in a way that makes them clearly competitive with the preconditioned implicit Newton–Krylov methods. In this paper we present a new class of implicit-exponential (IMEXP) methods which can both take advantage of efficient preconditioners developed for given operators and improve computational efficiency for problems where both operators L and N in (1.1) are stiff. The idea of combining an implicit treatment of operator L and an exponential approach to integrate the term with N was first proposed in [20] where a classically accurate second order IMEXP method was constructed. Here we expand this approach to derive several types of IMEXP integrators and provide derivation of stiffly accurate schemes along with the convergence theory for these methods. While we propose two main classes of integrators – IMEXP Runge–Kutta and hybrid IMEXP schemes – the ideas behind these methods can be used to construct many additional schemes that would address particular structure of the problem (1.1).

The paper is organized as follows. Section 2 outlines the main ideas behind construction of IMEXP schemes and presents the analytical framework that enables us to derive the stiff order conditions and to prove stability and convergence of the schemes. Construction and analysis of IMEXP Runge–Kutta methods is presented in Section 3 and development of hybrid IMEXP schemes is the focus of Section 4. Section 5 contains numerical experiments that validate theoretical results and illustrate computational savings that IMEXP methods can bring compared to IMEX schemes for problems with stiff N.

2. Construction and analytical framework for analysis of the IMEXP methods

We begin the construction of IMEXP methods by considering the general EPIRK framework introduced in [21]. The exponential propagation iterative methods of Runge–Kutta type (EPIRK) to solve (1.1) can be written as

$$\begin{aligned} U_{ni} &= u_n + \alpha_{i1}\psi_{i1}(g_{i1}h_nA_{i1})h_nF(u_n) + h_n\sum_{j=2}^{i-1}\alpha_{ij}\psi_{ij}(g_{ij}h_nA_{ij})D_{nj}, \quad i=2,\dots,s, \\ u_{n+1} &= u_n + \beta_1\psi_{s+1,1}(g_{s+1,1}h_nA_{s+1,1})h_nF(u_n) + h_n\sum_{j=2}^{s}\beta_j\psi_{s+1j}(g_{s+1,j}h_nA_{s+1,j})D_{n,s+1}, \end{aligned} \tag{2.1}$$

where u_n is an approximation to the solution of (1.1) at time $t_n = t_0 + \sum_{i=1}^{n} h_i$ and vectors D_{nj} typically depend on the stage values U_{ni}. As explained in [21,20,22], different choices for functions ψ_{ij}, matrices A_{ij} and vectors D_{nj} result in different classes of EPIRK methods. To construct IMEXP methods we can use the flexibility of EPIRK framework and choose ψ_{ij}, A_{ij} and D_{nj} to address the structure of the problem (1.1). Namely, we construct methods of two types – IMEXP Runge–Kutta and hybrid IMEXP schemes. The main idea behind both classes of methods is to choose some of the functions ψ_{ij} to be rational functions, similar to implicit or IMEX methods. The remaining ψ_{ij} are then set as linear combination of the exponential-like functions $\varphi_k(z)$ defined by