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A posteriori error estimation for multi-stage Runge–Kutta IMEX schemes

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ABSTRACT

Implicit–Explicit (IMEX) schemes are widely used for time integration methods for approximating solutions to a large class of problems. In this work, we develop accurate *a posteriori* error estimates of a quantity-of-interest for approximations obtained from multi-stage IMEX schemes. This is done by first defining a finite element method that is nodally equivalent to an IMEX scheme, then using typical methods for adjoint-based error estimation. The use of a nodally equivalent finite element method allows a decomposition of the error into multiple components, each describing the effect of a different portion of the method on the total error in a quantity-of-interest.

1. Introduction

In this paper we consider *a posteriori* error analysis for multi-stage implicit–explicit (IMEX) schemes applied to autonomous nonlinear ODEs,

$$\begin{cases} \dot{y}(t) = f(y(t)) + g(y(t)), \quad t \in (0, T], \\ y(0) = y_0. \end{cases} \tag{1}$$

Here $y(t) \in \mathbb{R}^m$, $\dot{y} = dy/dt$ and $f, g : \mathbb{R}^m \to \mathbb{R}^m$. The right hand side of (1) is split such that g represents a much smaller time scale than f, and is often referred to as the "stiff" term. Systems of the form (1) often arise from spatial discretization of partial differential equations, for example, convection–diffusion–reaction equations, and hyperbolic systems with relaxation [31], where f represents the convection term and g represents the diffusion or relaxation term.

As opposed to *a priori* error bounds, *a posteriori* error estimates provide an accurate computation of the discretization error in a particular approximation. Accurate error estimation is a critical component of numerical simulations, being useful for reliability, uncertainty quantification and adaptive error control. In particular, we consider goal-oriented *a posteriori* error estimation. Often, the aim of a numerical simulation is to compute the value of a linear functional of the solution, a so called quantity-of-interest (QoI) defined as,

$$Q(y) \equiv (y(T), \psi), \tag{2}$$

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where $\psi \in \mathbb{R}^m$ and $(\cdot,\cdot)$ denotes the standard Euclidean inner product. In this paper we employ adjoint based *a posteriori* analysis to quantify error for a given QoI. Adjoint based error estimation is widely used for a host of numerical methods including finite elements, time integration, multi-scale simulations and inverse problems [20,19,21,1,4,5,8,22,10,13,15,34]. The error estimate weights computable residuals of the numerical solution with the solution of an adjoint problem to quantify the accumulation and propagation of error. Moreover, the estimate also identifies different contributions to the total error.

Developing accurate and stable time integration of systems of the form (1) is challenging as the term g represents time scales which are often order of magnitudes smaller than the time scales for the component f [32]. IMEX schemes offer an attractive option for such systems. These schemes treat the f component explicitly while treating the g component implicitly. Hence, such schemes attempt to minimize the computational cost by balancing the number of nonlinear solves needed for an implicit scheme with the small time step required to maintain stability with an explicit scheme.

IMEX schemes are widely used for time integration methods for approximating solutions to a large class of problems [32,26,17,28,27,37,30,35,2,3,12,16,11,39,38]. IMEX schemes may be divided into two classes: multi-step IMEX schemes and multi-stage Runge–Kutta IMEX schemes (also termed here IMEX RK). Multi-step IMEX schemes are a generalization of multi-step schemes like Adams–Bashforth or backward differentiation formulas (BDF) and utilize solution values from previous time nodes to form the solution at the current time node. IMEX multi-step methods can be designed with various stability properties such as A-stability, L-stability and strong-stability preservation (SSP) that are desirable for a wide range of challenging systems [26]. Due to the inherent data dependencies of higher-order multi-step methods these techniques often require start-up procedures that employ lower-order approximations with smaller scaled time-step sizes to ramp up to the full formal approximation order. Additionally, to restart a calculation, additional old time step values for the solution are required. In contrast multi-stage Runge–Kutta in general, and multi-stage IMEX RK schemes specifically do not require ramping procedures and are self-restarting methods. This is a desirable feature for long-time-scale integrations with high-order accuracy. Additionally, multi-stage IMEX RK methods can also be designed with various stability properties such as A-stability, L-stability and strong-stability preservation (SSP) [26]. For an extensive comparison of multistep and multi-stage IMEX methods see [26] and the references contained therein. In general both IMEX multi-step and multi-stage methods have significant advantages and potential limitations when considering issues such as stability, accuracy, memory usage, restarting, etc. for specific classes of challenging multiphysics systems. However the ability to allow both explicit and implicit evaluation of operators in a multiple-time-scale multiphysics system integration, in a well structured general mathematical method, is very appealing as described above. This paper focuses on what we believe is the first development of quantity-of-interest focused *a posteriori* error estimation for IMEX RK type methods and complements our earlier work on IMEX multistep methods [13].

Adjoint-based *a posteriori* error estimation is widely applied to finite element approximations, as a variational formulation is needed to compute the error, however, there is some recent work which considers finite difference methods. Explicit multi-stage and multi-step time integrators are considered in [15] and multi-step IMEX schemes were considered in [13]. Error estimates for the Lax–Wendroff scheme were developed in [14] and certain Godunov methods were analyzed in [6,7,29].

In this paper, we derive *a posteriori* error estimates for the multi-stage Runge–Kutta IMEX schemes. To derive an estimate, we must first represent the scheme as a finite element method. This is done by developing a finite element method that is "nodally equivalent" to a certain IMEX scheme. A nodally equivalent finite element approximation agrees with the IMEX approximation at the discretization nodes, while still being defined on the entire temporal domain. The error representation formula is then derived using well defined methods. In addition, we decompose the error estimate into components representing different contributions to the error. In this way we are able to discuss the contribution of the implicit and explicit portions of the method to the total error in the quantity-of-interest.

The paper is organized as follows. In §2 we discuss the Runge–Kutta IMEX schemes and formulate an equivalent finite element method. This equivalence allows us to carry out *a posteriori* analysis in §3. Numerical examples arising from the discretization of partial differential equations are presented in §4. The examples are associated with linear and nonlinear convection diffusion type systems, a nonlinear Burger's equation with dissipation, and a coupled system from magnetohydrodynamics (MHD) representing propagation of an Alfvén wave in a viscous conducting fluid.

2. Preliminaries and equivalent finite element method

In this section, we introduce some notation, then give a brief review of generic ν-stage IMEX Runge–Kutta schemes. For a more complete discussion see [31,32,3]. Generic continuous Galerkin finite element methods are introduced for solving (1), and then the idea of nodal equivalency is explained and the equivalent finite element method is derived. Convergence properties of finite element methods for time integration are discussed in [19]. The section is concluded by showing second order convergence of the nodally equivalent finite element solution.

2.1. Notation and generic IMEX Runge–Kutta schemes

We begin with some notation. All approximations discussed are based on a discretization defined by the nodes

$$0 = t_0 < t_1 < \ldots < t_n < \ldots < t_N = T,$$