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Beyond conventional Runge–Kutta methods in numerical integration of ODEs and DAEs by use of structures and local models☆

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Abstract

There are two parts in this paper. In the first part we consider an overdetermined system of differential-algebraic equations (DAEs). We are particularly concerned with Hamiltonian and Lagrangian systems with holonomic constraints. The main motivation is in finding methods based on Gauss coefficients, preserving not only the constraints, symmetry, symplecticness, and variational nature of trajectories of holonomically constrained Hamiltonian and Lagrangian systems, but also having optimal order of convergence. The new class of (s, s)-Gauss–Lobatto specialized partitioned additive Runge–Kutta (SPARK) methods uses greatly the structure of the DAEs and possesses all desired properties. In the second part we propose a unified approach for the solution of ordinary differential equations (ODEs) mixing analytical solutions and numerical approximations. The basic idea is to consider local models which can be solved efficiently, for example analytically, and to incorporate their solution into a global procedure based on standard numerical integration methods for the correction. In order to preserve also symmetry we define the new class of symmetrized Runge–Kutta methods with local model (SRKLM).

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1. Introduction

In the first part of this paper we consider an overdetermined system of differential-algebraic equations (DAEs), see Section 2. We are particularly concerned with Hamiltonian and Lagrangian systems with holonomic constraints. The main motivation is in finding methods based on Gauss coefficients, preserving not only the constraints, symmetry, symplecticness, and variational nature of trajectories of holonomically constrained Hamiltonian and Lagrangian systems, but also having optimal order of convergence. When applied to nonstiff ordinary differential equations (ODEs), Gauss methods have maximal order of convergence in the class of RK methods. However, for index 3 DAEs, standard Gauss methods, are either divergent or have very low order of convergence. Gauss methods have thus not been considered

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of much practical interest for the numerical solution of high index DAEs in general. In this paper, we propose some modifications to the application of standard RK methods to index 3 DAEs in order to obtain methods with maximal order of convergence. The modifications that we propose have negligible computational cost. The new class of (s, s)-Gauss–Lobatto specialized partitioned additive Runge–Kutta (SPARK) methods is described in Section 3 and makes great use of the structure of the DAEs. The new schemes are constraint-preserving and symmetric. In Section 4, we show that for Hamiltonian and Lagrangian systems with holonomic constraints these schemes preserve symplecticness of the flow and that they satisfy a discrete variational principle: discrete trajectories are stationary with respect to a discrete action.

In the second part of this paper, we propose a unified approach for the solution of ODEs mixing analytical solutions and numerical approximations. When considering a system of ODEs and a given initial value, ideally one would like to obtain directly and explicitly its analytical solution. This is of course generally not possible. In the absence of an explicit analytical solution, one is generally left with two approximation tools: perturbation techniques and numerical integration methods. Perturbation techniques are primarily based on asymptotic expansions. These techniques require at least the analytical solution of a nearby problem, they are often highly technical and they can be applied only to specific situations. For most systems perturbation techniques are not applicable with ease and one is left to solve the problem numerically. In contrast to perturbation techniques, numerical integration methods do not generally incorporate the use of any analytical solution of a nearby problem even when it is available. One aim of this paper is to reconcile both analytical and numerical approaches by giving unified procedures mixing analytical solutions of local models together with numerical approximations in order to find the solution of the original problem more efficiently. This is an idea analogous to the goal of preconditioning when solving linear systems of equations with iterative methods. Mixing analytical solutions of local models with numerical approximations has some advantages. First of all, for a given standard numerical method it generally reduces the error and thus allows to take larger stepsizes. Secondly it allows the development of multiscale procedures based on hierarchical models. The idea of mixing analytical solutions together with numerical methods is certainly not new, but it has not been much explored and fully exploited in ODEs and DAEs. We note that there has been some renewed interest on exponential methods [6,8,15,16], i.e., on methods using the exact solution of linear ODEs. In this paper, we propose a more general approach applicable to different kind of problems and not limited to linear models. The basic idea is to consider local models which can be solved efficiently, for example analytically, and to incorporate their solution into a global procedure based on standard numerical integration methods for the correction, see Section 5. In order to also preserve symmetry we define the new class of symmetrized Runge–Kutta methods with local model (SRKLM) in Section 6. In Section 7 we give some numerical experiments to illustrate some of the theoretical results.

2. A system of implicit differential-algebraic equations

We consider the following class of systems of implicit DAEs

$$\frac{\mathrm{d}}{\mathrm{d}t} q(t, y) = v(t, y, z), \tag{1a}$$

$$\frac{\mathrm{d}}{\mathrm{d}t} p(t, y, z) = f(t, y, z) + r(t, y, \psi), \tag{1b}$$

$$0 = g(t, y). \tag{1c}$$

Differentiating the constraints (1c) once with respect to t leads to

$$0 = g_t(t, y) + g_y(t, y)(q_y(t, y))^{-1}(v(t, y, z) - q_t(t, y)). \tag{1d}$$

In mechanics the quantities q, v, p, f, and r represent, respectively, generalized coordinates, generalized velocities, generalized momenta, generalized forces, and reaction forces due to the constraints (1c) [7,20]. The variable $t \in \mathbb{R}$ is the independent variable, the variables $y \in \mathbb{R}^{n_y}$ and $z \in \mathbb{R}^{n_z}$ are called the *differential* variables, and the variables $\psi \in \mathbb{R}^{n_\psi}$ are called the *algebraic* variables. The latter correspond to Lagrange multipliers when the DAEs are derived from some constrained variational principle [7,20]. We have $q \in \mathbb{R}^{n_y}$, $p \in \mathbb{R}^{n_z}$, $g \in \mathbb{R}^{n_\psi}$, $v \in \mathbb{R}^{n_y}$, $f \in \mathbb{R}^{n_z}$, and $r \in \mathbb{R}^{n_z}$. Some differentiability conditions on the above functions and consistency of the initial values y_0, z_0, ψ_0 at