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Using additivity in numerical integration of DAEs

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We report on extensions of Gauss methods and the Hilber-Hughes-Taylor (HHT) method for differential-algebraic equations (DAEs) arising in mechanics.

Gauss methods have not been considered as having much practical interest for the numerical solution of DAEs. This has been mainly due to poor convergence properties of these methods when applied in a standard direct way. Stiffly accurate methods have generally better convergence properties to solve DAEs [1, 3, 5]. However, in the context of geometric numerical integration of ODEs, e.g., for Hamiltonian or Lagrangian systems, Gauss methods have excellent theoretical properties [2]. It was an open problem and a question of interest to know if there was any way of generalizing and developing methods based on Gauss coefficients that would lead to methods of high order and quality for DAEs while preserving geometric properties of DAEs. It was shown recently that such generalizations are indeed possible for DAEs of index 2 [6, 10] and index 3 [7, 8].

Let us consider DAEs of the form

$$y' = v(t,y,z), \tag{1a}$$

$$(p(t,y,z))' = f(t,y,z) + r(t,y,\psi), \tag{1b}$$

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

where in mechanics the quantities y, v, p, f, and r represent respectively generalized coordinates, generalized velocities, generalized momenta, generalized forces, and reaction forces due to the holonomic constraints $g(t,y) = 0$ ($r(t,y,\psi) = -g_y^T(t,y)\psi$). Differentiating (1c) once one obtains additional velocity constraints

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

The matrices $p_z(t,y,z)$ and $g_y(t,y)v_z(t,y,z)p_z^{-1}(t,y,z)r_\psi(t,y,\psi)$ are assumed to be invertible. The above formulation generalizes both Hamiltonian ($p = z$) and Lagrangian systems ($v = z$) with holonomic constraints. Applied to the system (1) one step with stepsize h of the standard 1-stage Gauss RK method is divergent in general even when $p(t,y,z) = z$ and $r(t,y,\psi)$ is linear in the algebraic variables ψ.

The modified method based on the implicit midpoint rule that we propose reads

$$\begin{aligned}
Y_1 &= y_0 + \frac{h}{2} v(T_1, Y_1, Z_1), \\
p(T_1, Y_1, Z_1) &= p(y_0, z_0) + \frac{h}{2} f(T_1, Y_1, Z_1) + \frac{h}{2} r(t_0, y_0, \Psi_0), \\
y_1 &= y_0 + h v(T_1, Y_1, Z_1), \\
0 &= g(t_1, y_1), \\
p(t_1, y_1, z_1) &= p(t_0, y_0, z_0) + h f(T_1, Y_1, Z_1) + \frac{h}{2} r(t_0, y_0, \Psi_0) + \frac{h}{2} r(t_1, y_1, \Psi_1), \\
0 &= g_y(t_1, y_1) v(t_1, y_1, z_1),
\end{aligned}$$

where h is the stepsize, $T_1 := t_0 + h/2$, and $t_1 := t_0 + h$. We call this method the $(1,1)$-*Gauss-Lobatto specialized partitioned additive Runge-Kutta (SPARK) method*. It mixes coefficients from the midpoint rule with those from the trapezoidal rule to treat holonomic constraints properly. It makes use of the additivity of the differential equations (1b). Note that the quantity Ψ_0 above is an internal algebraic variable, it is not an initial condition or a value ψ_0 coming from the previous step. We can generalize these ideas to obtain higher order schemes based on Gauss coefficients mixed with Lobatto coefficients. The family of Gauss-Lobatto SPARK methods makes great use of the partitioning and additive structure of the equations (1). We summarize our findings in the following theorem [7, 8]:

Theorem 1: *For the overdetermined system of DAEs (1) the (s,s)-Gauss-Lobatto SPARK methods are constraint-preserving, symmetric, and of maximal order $2s$. For holonomically constrained Hamiltonian systems and Lagrangian systems these methods are also symplectic and variational.*

The HHT method is widely used in structural dynamics [4]. The HHT method for $y'' = f(t, y, y')$ or equivalently for

$$y' = z, \qquad z' = f(t, y, z),$$

can be expressed as an implicit non-standard one-step method as follows

$$\begin{aligned}
y_1 &= y_0 + h z_0 + \frac{h^2}{2} \left((1 - 2\beta) a_0 + 2\beta a_1 \right), \\
z_1 &= z_0 + h \left((1 - \gamma) a_0 + \gamma a_1 \right), \\
a_1 &= (1 + \alpha) f(t_1, y_1, z_1) - \alpha f(t_0, y_0, z_0),
\end{aligned}$$

where a_0 and a_1 are approximations to the acceleration $a(t) := f(t, y(t), z(t))$ at $t_0 + \alpha h$ and $t_1 + \alpha h$ respectively. The coefficients α, β, γ are taken according to $\alpha \in [-1/3, 0], \beta = (1 - \alpha)^2/4, \gamma = 1/2 - \alpha$. We have extended the HHT method to the DAEs (1) with $v = p = z$, i.e., to DAEs of the form

$$(2) \quad y' = z, \quad z' = f(t, y, z) + r(t, y, \psi), \quad 0 = g(t, y), \quad 0 = g_t(t, y) + g_y(t, y) z.$$

Given (y_0, z_0, a_0) we define the extended HHT method for (2) as follows

$$\text{(3a)} \quad y_1 = y_0 + hz_0 + \frac{h^2}{2}\left((1-2\beta)a_0 + 2\beta a_1\right) + \frac{h^2}{2}((1-b)R_0 + bR_1),$$

$$\text{(3b)} \quad z_1 = z_0 + h\left((1-\gamma)a_0 + \gamma a_1\right) + \frac{h}{2}\left(R_0 + R_1\right),$$

$$\text{(3c)} \quad a_1 = (1+\alpha)f(t_1, y_1, z_1) - \alpha f(t_0, y_0, z_0),$$

where $b \neq 1/2$ is a new free coefficient,

$$\text{(3d)} \qquad R_0 = r(t_0, y_0, \Psi_0), \qquad R_1 = r(t_1, y_1, \Psi_1),$$

and Ψ_0 is not a value ψ_0 coming from the previous step or an initial condition, but Ψ_0 and Ψ_1 are internal algebraic variables determined by the two sets of constraints

$$\text{(3e)} \qquad 0 = g(t_1, y_1), \qquad 0 = g_t(t_1, y_1) + g_y(t_1, y_1)z_1.$$

Once again we make use of the additivity of the differential equations for z' in (2). To make the method less implicit, one can replace R_1 by $r(t_1, y_0 + hz_0, \Psi_1)$ in (3d). Theorem 2 below remains valid in this situation. One can show global convergence of order 2 of the extended HHT method [9]:

Theorem 2: *Consider the overdetermined system of DAEs (2) with initial conditions (y_0, z_0, a_0) at t_0 satisfying*

$$g(t_0, y_0) = 0, \quad g_t(t_0, y_0) + g_y(t_0, y_0)z_0 = 0, \quad a_0 - a(t_0 + \alpha h) = O(h).$$

Then the numerical solution (y_n, z_n, a_n) at t_n to the system of equations (3) satisfies for $0 \leq h \leq h_0$ and $t_n - t_0 = nh \leq Const$

$$y_n - y(t_n) = O(h^2), \qquad z_n - z(t_n) = O(h^2), \qquad a_n - a(t_n + \alpha h) = O(h^2),$$

where $(y(t), z(t))$ is the exact solution to (1) at t passing through (y_0, z_0) at t_0.

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Explicit, volume preserving splitting methods for divergence-free polynomial vector fields

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(joint work with Robert I. McLachlan, Hans Z. Munthe-Kaas and G. R. W. Quispel)

In this talk we address the problem of the numerical integration of divergence-free vector fields by volume-preserving methods. It is well known that devising methods which preserve volume is quite a hard task. To-date the general techniques consist in splitting the given vector field into the sum of two-dimensional volume-preserving systems and solve those by symplectic methods (Feng Kang) or by solving for $n-1$ variables and then correct for the last one in order to obtain a volume-preserving method (Shang Zai-jiu, 1994, Quispel 1995). However, these methods are generally implicit and expensive. Explicit methods exist for particular problems, for instance trigonometric ones.

We address the case of polynomial vector fields.

The main idea is to split the given divergence free vector field into the sum of pieces that

- Can be integrated exactly easily, or
- Can be integrated in a volume preserving manner by simple explicit methods (a.k.a. Forward Euler) and whose adjoint is also explicit.

Then, the basic split terms can be combined to obtain higher order integrator, either by Yoshida's technique, or by other symmetric composition methods.

Several new methods are presented for linear and quadratic problems. Roughly, these can be divided into two classes: i) methods that distinguish the diagonal part (all the terms in equation i that include the variable x_i, for $i = 1, 2 \ldots, n$), and ii) methods that do not distinguish the diagonal part. The diagonal part is generally more difficult to treat as its coefficient are interconnected as a result of volume-preservation, however it is computationally less expensive, as the off-diagonal part requires computations of a order of n higher.

Among the methods for the diagonal part, we mention the splitting in d shears, where d is the degree of the polynomial vector field, and exponentiation. As for the off-diagonal part, we consider splitting in strictly lower triangular systems (as these can be integrated in a volume-preserving manner by any Runge–Kutta method) by permutations, as well as splitting in n natural shears, which are integrated exactly by a step of Forward Euler. As for methods that do not distinguish the diagonal part, we consider a splitting in $n + d$ shears. The splitting in shears has been