**CONSISTENT EXTENSIONS OF THE SYMPLECTIC EULER METHOD FOR A CLASS OF OVERDETERMINED DAES.**

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**Abstract.** The symplectic Euler method applied to Hamiltonian systems with holonomic constraints is known to preserve the symplectic structure of the flow on the constraint manifold. We consider two extensions of this method to a class of overdetermined differential-algebraic equations (ODAEs) arising in mechanics. It is shown that a natural extension of the symplectic Euler method is inconsistent for ODAEs which are nonlinear in the algebraic variables. A different non-trivial extension is given and shown to be consistent. Our results are confirmed numerically on two test problems. One test problem is a model of a mass moving on a surface with a nonlinearity in the Lagrange multiplier.

**Key words.** Differential-algebraic equations, differential-algebraic inequalities, Hamiltonian systems, symplectic Euler.

**AMS subject classifications.** 65L05, 65L06, 65L80, 70F20, 70H03, 70H05, 70H45.

**1. Introduction.** The symplectic Euler method applied to Hamiltonian systems with holonomic constraints is known to be symplectic [2, 4, 8]. The purpose of this short paper is to better understand the nature of this method and to extend it to a class of overdetermined differential-algebraic equations (ODAEs), for example in the presence of friction [7]. A generalization of the symplectic Euler method called the 'natural' symplectic Euler method, is shown to be inconsistent for ODAEs which are nonlinear in the algebraic variables. A different non-trivial generalization of the symplectic Euler method, called the 'true' symplectic Euler method is defined and shown to be consistent and convergent. The algorithm given can be the basis of higher order methods obtained by composition [2]. The ideas given in this paper can also be applied to various combinations of the explicit Euler and implicit Euler methods as well. Such methods can be the basis of time-stepping algorithms for the solution of overdetermined differential-algebraic inequalities (ODAIs) which form an important class of nonsmooth/discontinuous dynamical systems [1].

This paper is organized as follows. In section 2 we introduce the equations of Hamiltonian systems with holonomic constraints and the definition of the symplectic Euler method. In section 3 we consider extensions of the symplectic Euler method to a class of ODAEs. The 'natural', 'true', and 'conjugate' symplectic Euler methods are defined and analyzed. Two numerical experiments are given in section 4 to illustrate our theoretical results. One test problem is a model of a mass moving on a surface with a nonlinearity in the Lagrange multiplier. Finally a short conclusion is given in section 5.

**2. The symplectic Euler method for Hamiltonian systems with holonomic constraints.** The Hamiltonian system with Hamiltonian $H : \mathbb{R}^d \times \mathbb{R}^d \longrightarrow \mathbb{R}$ and holonomic constraints $g : \mathbb{R}^d \longrightarrow \mathbb{R}^{d_g}$ $(d_g < d)$ is given by

$$\frac{d}{dt}q = \nabla_p H(q,p), \tag{2.1a}$$

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$$\frac{d}{dt}p = -\nabla_q H(q,p) - g_q^T(q)\lambda, \tag{2.1b}$$

$$0 = g(q), \tag{2.1c}$$

$$0 = g_q(q)\nabla_p H(q,p). \tag{2.1d}$$

In mechanics the quantities $q \in \mathbb{R}^d, p \in \mathbb{R}^d$ usually represent respectively generalized coordinates and generalized momenta. The equation (2.1d) follows from (2.1c) as a consequence of $0 = \frac{d}{dt}g(q) = g_q(q)\frac{d}{dt}q$ and (2.1a). Well-known properties of Hamiltonian systems with holonomic constraints are as follows:

1. The Hamiltonian is invariant along a solution, i.e.,

$$H(q(t),p(t)) = Const.$$

2. The flow $\phi_\tau : (q(t),p(t))) \mapsto (q(t+\tau),p(t+\tau))$ of (2.1) preserves the symplectic 2-form

$$\omega = \sum_{i=1}^{d} dq^i \wedge dp^i$$

on $V := \left\{(q,p) \in \mathbb{R}^d \times \mathbb{R}^d \mid 0 = g(q),\ 0 = g_q(q)H_p(q,p)\right\}$, i.e., the flow is *symplectic* on $V$.

3. For $\ell(q,p) := p^T\nabla_p H(q,p) - H(q,p)$ the action of the Hamiltonian

$$\int_{t_a}^{t_b} \ell(q(t),p(t)) - g^T(q(t))\lambda(t)dt,$$

is stationary. This is Hamilton's variational principle.

The *symplectic Euler method* applied to (2.1) is defined as follows [2, 4, 8]

$$P_1 = p_0 - h\nabla_q H(q_0,P_1) - hg_q^T(q_0)\Lambda_0, \tag{2.2a}$$

$$q_1 = q_0 + h\nabla_p H(q_0,P_1), \tag{2.2b}$$

$$0 = g(q_1), \tag{2.2c}$$

$$\begin{aligned} p_1 &= p_0 - h\nabla_q H(q_0,P_1) - hg_q^T(q_0)\Lambda_0 - hg_q^T(q_1)\Lambda_1 \\ &= P_1 - hg_q^T(q_1)\Lambda_1, \end{aligned} \tag{2.2d}$$

$$0 = g_q(q_1)\nabla_p H(q_1,p_1). \tag{2.2e}$$

It is a method of order 1 and the two quantities $\Lambda_0$, $\Lambda_1$ are locally determined by these equations. This method is known to be symplectic [4, 8] and to be variational in the sense of Marsden and West [6]. This also follows directly from results given in [5] since this method can be interpreted as a specialized partitioned additive Runge-Kutta (SPARK) method.

**3. Extending the symplectic Euler method to a class of ODAEs.** We are interested in extending this method to the following system of ODAEs

$$\frac{d}{dt}y = v(y,z), \tag{3.1a}$$

$$\frac{d}{dt}z = f(y,z) + r(y,z,\psi), \tag{3.1b}$$

$$0 = g(y), \tag{3.1c}$$

$$0 = g_y(y)v(y,z), \tag{3.1d}$$

where $r(y,z,\psi)$ may be nonlinear in $\psi$. We assume $y \in \mathbb{R}^{d_y}$, $z \in \mathbb{R}^{d_z}$, $\psi \in \mathbb{R}^{d_g}$, and $g : \mathbb{R}^{d_y} \longrightarrow \mathbb{R}^{d_g}$ $(d_g < d_y)$. The equation (3.1d) follows from $0 = \frac{d}{dt} g(y) = g_y(y) \frac{d}{dt} y$ and (3.1a). Any solution must lie on the manifold of constraints

$$\mathcal{M} := \left\{ (y,z) \in \mathbb{R}^{d_y} \times \mathbb{R}^{d_z} \mid 0 = g(y),\ 0 = g_y(y) v(y,z) \right\}.$$

For consistent initial values, i.e., for $(y_0, z_0) \in \mathcal{M}$ we have existence and uniqueness of a solution under the assumption that

$$g_y(y) v_z(y,z) r_\psi(y,z,\psi) \quad \text{is invertible} \tag{3.1e}$$

in a neighborhood of the solution. The whole system (3.1) can be considered as a system of index 2 ODAEs. Of course such a general system of ODAEs does not possess any symplectic structure in general. For Hamiltonian systems with holonomic constraints (2.1) we have $y = q$, $z = p$, $\psi = \lambda$, $v(y,z) = \nabla_z H(y,z)$, $f(y,z) = -\nabla_y H(y,z)$, and $r(y,z,\psi) = -g_y(y)^T \psi$. The results given in this paper can be extended to Lagrangian systems with holohomic constraints and more generally to systems where $\frac{d}{dt} z$ in (3.1b) is replaced by $\frac{d}{dt} p(y,z)$ and such that $p_z$ is nonsingular, see [5].

**3.1. The 'natural' symplectic Euler method.** A *'natural'* extension of (2.2) to (3.1) is given by

$$\begin{aligned}
&(3.2a) && Z_1 = z_0 + hf(y_0, Z_1) + h\alpha r(y_0, z_0, \Psi_0),\\
&(3.2b) && y_1 = y_0 + hv(y_0, Z_1),\\
&(3.2c) && 0 = g(y_1),\\
&(3.2d) && z_1 = z_0 + hf(y_0, Z_1) + h\alpha r(y_0, z_0, \Psi_0) + h(1-\alpha) r(y_1, z_1, \Psi_1)\\
& && \quad = Z_1 + h(1-\alpha) r(y_1, z_1, \Psi_1),\\
&(3.2e) && 0 = g_y(y_1) v(y_1, z_1),
\end{aligned}$$

with $\alpha \neq 0, 1$ (e.g., $\alpha = 1/2$ corresponds to the use of the trapezoidal rule) to ensure existence and uniqueness of the numerical solution. This is the extension and interpretation of the symplectic Euler method (2.2) as a specialized partitioned additive Runge-Kutta (SPARK) method [5]. Notice that in the original symplectic Euler method (2.2) the quantities $\Lambda_0$ and $\Lambda_1$ correspond to $\Lambda_0 = \alpha \Psi_0$ and $\Lambda_1 = (1-\alpha)\Psi_1$. We have the following result:

THEOREM 3.1. *For (3.1) when $r(y,z,\psi)$ is nonlinear in $\psi$, the 'natural' symplectic Euler (3.2) is inconsistent (i.e., of order 0), and we have only $z_1 - z(t_0+h) = O(h)$ even if $r(y,z,\psi) = r(\psi)$ is independent of $y$ and $z$. However, when $r(y,z,\psi)$ is affine in $\psi$, it is consistent (i.e., of order at least 1), and we have $z_1 - z(t_0+h) = O(h^2)$.*

*Proof.* To emphasize the dependence of $\Psi_0$ and $\Psi_1$ on $h$ we denote these two quantities by $\Psi_0(h)$ and $\Psi_1(h)$. From (3.2a) we have

$$Z_1 = z_0 + h(f(y_0, z_0) + \alpha r(y_0, z_0, \Psi_0(h))) + O(h^2).$$

Hence, from (3.2b) we get

$$y_1 = y_0 + hv(y_0, z_0) + h^2 v_z(y_0, z_0)(f(y_0, z_0) + \alpha r(y_0, z_0, \Psi_0(h))) + O(h^3).$$

From (3.2c) this leads to

$$0 = \frac{1}{h^2} g(y_1)$$

$$= \frac{1}{h^2} g(y_0) + \frac{1}{h} g_y(y_0)v(y_0,z_0) + g_y(y_0)v_z(y_0,z_0)(f(y_0,z_0) + \alpha r(y_0,z_0,\Psi_0(h))) + \frac{1}{2} g_{yy}(y_0)(v(y_0,z_0),v(y_0,z_0)) + O(h).$$

Assuming $g(y_0) = 0$ and $g_y(y_0)v(y_0,z_0) = 0$, the value $\Psi_0(0) := \lim_{h\to 0}\Psi_0(h)$ must satisfy

$$0 = g_y(y_0)v_z(y_0,z_0)(f(y_0,z_0) + \alpha r(y_0,z_0,\Psi_0(0))) + \frac{1}{2} g_{yy}(y_0)(v(y_0,z_0),v(y_0,z_0)). \tag{3.3}$$

Therefore, $\Psi_0(0) \neq \psi_0$ where $\psi_0$ is the consistent value satisfying the underlying constraint corresponding to $0 = \frac{d}{dt}(g_y(y)v(y,z))$

$$0 = g_{yy}(y)(v(y,z),v(y,z)) + g_y(y)v_y(y,z)v(y,z) + g_y(y)v_z(y,z)(f(y,z) + r(y,z,\psi))$$

at $(y_0,z_0,\psi_0)$. From (3.2d) we have

$$z_1 = z_0 + h(f(y_0,z_0) + \alpha r(y_0,z_0,\Psi_0(h)) + (1-\alpha)r(y_0,z_0,\Psi_1(h))) + O(h^2).$$

From (3.2e) this leads to

$$\begin{aligned} 0 &= \frac{1}{h} g_y(y_1)v(y_1,z_1) \\ &= \frac{1}{h} g_y(y_0)v(y_0,z_0) + g_{yy}(y_0)(v(y_0,z_0),v(y_0,z_0)) + g_y(y_0)v_y(y_0,z_0)v(y_0,z_0) \\ &\quad + g_y(y_0)v_z(y_0,z_0)(f(y_0,z_0) + \alpha r(y_0,z_0,\Psi_0(h)) + (1-\alpha)r(y_0,z_0,\Psi_1(h))) + O(h). \end{aligned}$$

Assuming $g_y(y_0)v(y_0,z_0) = 0$, the value $\Psi_1(0) := \lim_{h\to 0}\Psi_1(h)$ must satisfy

$$\begin{aligned} 0 &= g_{yy}(y_0)(v(y_0,z_0),v(y_0,z_0)) + g_y(y_0)v_y(y_0,z_0)v(y_0,z_0) \\ &\quad + g_y(y_0)v_z(y_0,z_0)(f(y_0,z_0) + \alpha r(y_0,z_0,\Psi_0(0)) + (1-\alpha)r(y_0,z_0,\Psi_1(0))). \end{aligned} \tag{3.4}$$

Hence, taking (3.3) into account, $\Psi_1(0)$ must satisfy

$$\begin{aligned} 0 &= \frac{1}{2} g_{yy}(y_0)(v(y_0,z_0),v(y_0,z_0)) + g_y(y_0)v_y(y_0,z_0)v(y_0,z_0) \\ &\quad + g_y(y_0)v_z(y_0,z_0)(1-\alpha)r(y_0,z_0,\Psi_1(0)). \end{aligned}$$

Therefore, in general $\Psi_1(0) \neq \psi_0$, i.e., $\Psi_1(0)$ is also inconsistent. Hence, in general

$$\lim_{h\to 0} (\alpha r(y_0,z_0,\Psi_0(h)) + (1-\alpha)r(y_1(h),z_1(h),\Psi_1(h))) = \alpha r(y_0,z_0,\Psi_0(0)) + (1-\alpha)r(y_0,z_0,\Psi_1(0)) \neq r(y_0,z_0,\psi_0).$$

Thus,

$$z_1 = z_0 + h(f(y_0,z_0) + \alpha r(y_0,z_0,\Psi_0(0)) + (1-\alpha)r(y_0,z_0,\Psi_1(0))) + O(h^2)$$

and since

$$z(t_0+h) = z_0 + h(f(y_0,z_0) + r(y_0,z_0,\psi_0)) + O(h^2),$$

we have $z_1 - z(t_0+h) = O(h)$. Nevertherless, when $r(y,z,\psi)$ affine in $\psi$ (i.e., $r(y,z,\psi) = r_0(y,z) + r_\psi(y,z)\psi$), the method is of order 1 since

$$\alpha r(y_0,z_0,\Psi_0(0)) + (1-\alpha)r(y_0,z_0,\Psi_1(0)) = r(y_0,z_0,\alpha\Psi_0(0) + (1-\alpha)\Psi_1(0)),$$

$\alpha\Psi_0(0)+(1-\alpha)\Psi_1(0)$ is consistent by (3.4), i.e., we have $\alpha\Psi_0(0)+(1-\alpha)\Psi_1(0) = \psi_0$. Therefore, in the situation where $r(y,z,\psi)$ is affine in $\psi$ we have

$$\alpha r(y_0, z_0, \Psi_0(0) + (1-\alpha) r(y_0, z_0, \Psi_1(0)) = r(y_0, z_0, \psi_0),$$

leading to $z_1 - z(t_0 + h) = O(h^2)$. □

From the proof above, we note that for (2.2) a consistent approximation to the Lagrange multipliers $\lambda(t_0 + h)$ is given by $\Lambda_0 + \Lambda_1$ and not by $\Lambda_0$ or $\Lambda_1$.

A problem now is to find a consistent extension of the symplectic Euler method (2.2) to (3.1) when $r(y,z,\psi)$ is nonlinear in $\psi$. We give such an extension in the next section 3.2.

**3.2. The 'true' symplectic Euler method.** The inconsistency of the 'natural' symplectic Euler (3.2) in $z_1$ is due to an inconsistent value $\Psi_0(0)$. From (3.2d) we have

$$\begin{aligned} z_1 &= Z_1 - h\alpha r(y_1, z_1, \Psi_1) + hr(y_1, z_1, \Psi_1) \\ &= z_0 + hf(y_0, Z_1) + h\alpha(r(y_0, z_0, \Psi_0) - r(y_1, z_1, \Psi_1)) + hr(y_1, z_1, \Psi_1). \end{aligned}$$

To obtain a consistent value $z_1$ an idea is to replace the quantity $(r(y_0, z_0, \Psi_0) - r(y_1, z_1, \Psi_1))$ above by $(r(y_0, z_0, \Psi_0) - r(y_1, z_1, \Psi_0))$ which vanishes for $h \to 0$. We obtain then what we call the *'true'* symplectic Euler method

$$\begin{aligned} &(3.5a) \quad Z_1 = z_0 + hf(y_0, Z_1) + h\alpha r(y_0, z_0, \Psi_0), \\ &(3.5b) \quad y_1 = y_0 + hv(y_0, Z_1), \\ &(3.5c) \quad 0 = g(y_1), \\ &(3.5d) \quad z_1 = z_0 + hf(y_0, Z_1) + h\alpha(r(y_0, z_0, \Psi_0) - r(y_1, z_1, \Psi_0)) + hr(y_1, z_1, \widetilde{\Psi}_1) \\ &\qquad\quad\;\; = Z_1 - h\alpha r(y_1, z_1, \Psi_0) + hr(y_1, z_1, \widetilde{\Psi}_1), \\ &(3.5e) \quad 0 = g_y(y_1) v(y_1, z_1), \end{aligned}$$

with $\alpha \neq 0$ to ensure existence and uniqueness of the numerical solution. Note that our results below are still valid if we replace $z_0$ and $z_1$ in the $r$ terms of (3.5) indifferently by $z_0$, $z_1$, or $Z_1$.

THEOREM 3.2. *For (3.1), when $r(y,z,\psi)$ is nonlinear in $\psi$, the 'true' symplectic Euler method (3.5) is consistent of order* 1, *and we have $z_1 - z(t_0+h) = O(h^2)$. When $r(y,z,\psi)$ is affine in $\psi$ the 'true' symplectic Euler method (3.5) is equivalent to the 'natural' symplectic Euler (3.2). Hence, for Hamiltonian systems with holonomic constraints (2.1) the 'true' symplectic Euler method (3.5) is also symplectic and variational in the sense of Marsden and West.*

*Proof.* Following the proof of Theorem 3.1 we have from (3.5d)

$$z_1 = z_0 + h(f(y_0, z_0) + \alpha(r(y_0, z_0, \Psi_0(h)) - r(y_1, z_1, \Psi_0(h))) + r(y_1, z_1, \widetilde{\Psi}_1(h))) + O(h^2).$$

From (3.5e) this leads to

$$\begin{aligned} 0 &= \frac{1}{h} g_y(y_1) v(y_1, z_1) \\ &= \frac{1}{h} g_y(y_0) v(y_0, z_0) + g_{yy}(y_0)(v(y_0, z_0), v(y_0, z_0)) + g_y(y_0) v_y(y_0, z_0) v(y_0, z_0) \\ &\quad + g_y(y_0) v_z(y_0, z_0)(f(y_0, z_0) + \alpha(r(y_0, z_0, \Psi_0(h)) - r(y_1, z_1, \Psi_0(h))) + r(y_1, z_1, \widetilde{\Psi}_1(h))) \\ &\quad + O(h). \end{aligned}$$

Assuming $g_y(y_0)v(y_0,z_0)=0$, since

$$\lim_{h\to 0}\left(r(y_0,z_0,\Psi_0(h))-r(y_1,z_1,\Psi_0(h))\right)=r(y_0,z_0,\Psi_0(0))-r(y_0,z_0,\Psi_0(0))=0,$$

the value $\widetilde{\Psi}_1(0):=\lim_{h\to 0}\widetilde{\Psi}_1(h)$ must satisfy

$$\begin{aligned}0=&\,g_{yy}(y_0)(v(y_0,z_0),v(y_0,z_0))+g_y(y_0)v_y(y_0,z_0)v(y_0,z_0)\\&+g_y(y_0)v_z(y_0,z_0)(f(y_0,z_0)+r(y_0,z_0,\widetilde{\Psi}_1(0))).\end{aligned}$$

Therefore, $\widetilde{\Psi}_1(0)=\psi_0$ by local uniqueness. Thus,

$$\begin{aligned}z_1&=z_0+h(f(y_0,z_0)+\alpha(r(y_0,z_0,\Psi_0(0))-r(y_0,z_0,\Psi_0(0)))+r(y_0,z_0,\widetilde{\Psi}_1(0)))+O(h^2)\\&=z_0+h(f(y_0,z_0)+r(y_0,z_0,\psi_0))+O(h^2),\end{aligned}$$

and we have $z_1-z(t_0+h)=O(h^2)$.

When $r(y,z,\psi)$ is affine in $\psi$ the 'natural' symplectic Euler method (3.2) is equivalent to the 'true' symplectic Euler method (3.5) by considering the relation

$$\widetilde{\Psi}_1=\alpha\Psi_0+(1-\alpha)\Psi_1.$$

For (2.2) this corresponds to $\widetilde{\Psi}_1=\Lambda_0+\Lambda_1$. Hence, its symplecticness and its variational property follow directly since for (2.1) the 'natural' symplectic Euler method (3.2) is known to be symplectic and variational in the sense of Marsden and West see [4, 5, 6, 8]. □

For the modified Newton iterations to solve the nonlinear systems of equations (3.5), as an initial guess for the inconsistent unknown $\Psi_0$ we recommend not to use the value $\widetilde{\Psi}_1$ from the previous time step, but to use for example the value of $\Psi_0$ from the previous time step.

**3.3. The 'conjugate' symplectic Euler method.** For Hamiltonian systems with holonomic constraints (2.1) the conjugate symplectic Euler method is defined as follows

$$\begin{aligned}
&\text{(3.6a)} && P_1=p_0-hg_q^T(q_0)\Lambda_0,\\
&\text{(3.6b)} && q_1=q_0+h\nabla_pH(q_1,P_1),\\
&\text{(3.6c)} && 0=g(q_1),\\
&\text{(3.6d)} && p_1=p_0-h\nabla_qH(q_1,P_1)-hg_q^T(q_0)\Lambda_0-hg_q^T(q_1)\Lambda_1\\
&&& \quad=P_1-h\nabla_qH(q_1,P_1)-hg_q^T(q_1)\Lambda_1,\\
&\text{(3.6e)} && 0=g_q(q_1)\nabla_pH(q_1,p_1).
\end{aligned}$$

A similar analysis as above for the 'true' symplectic Euler method (3.5) can be carried out for this method. For (3.1) the 'true' conjugate symplectic Euler method can be defined as follows

$$\begin{aligned}
&\text{(3.7a)} && Z_1=z_0+h\alpha r(y_0,z_0,\Psi_0),\\
&\text{(3.7b)} && y_1=y_0+hv(y_1,Z_1),\\
&\text{(3.7c)} && 0=g(y_1),\\
&\text{(3.7d)} && z_1=z_0+hf(y_1,Z_1)+h\alpha r(y_0,z_0,\Psi_0)+h(1-\alpha)r(y_1,z_1,\Psi_1)\\
&&& \quad=Z_1+hf(y_1,Z_1)+h(1-\alpha)r(y_1,z_1,\Psi_1),\\
&\text{(3.7e)} && 0=g_y(y_1)v(y_1,z_1),
\end{aligned}$$

with $\alpha \neq 0, 1$. Notice that in the original conjugate symplectic Euler method (3.6) the quantities $\Lambda_0$ and $\Lambda_1$ correspond to $\Lambda_0 = \alpha\Psi_0$ and $\Lambda_1 = (1-\alpha)\Psi_1$. For (3.1) the 'true' conjugate symplectic Euler method can be defined as follows

$$
\begin{aligned}
&(3.8a) \qquad & Z_1 &= z_0 + h\alpha r(y_0, z_0, \Psi_0),\\
&(3.8b) \qquad & y_1 &= y_0 + hv(y_1, Z_1),\\
&(3.8c) \qquad & 0 &= g(y_1),\\
&(3.8d) \qquad & z_1 &= z_0 + hf(y_1, Z_1) + h\alpha(r(y_0, z_0, \Psi_0) - r(y_1, z_1, \Psi_0)) + hr(y_1, z_1, \widetilde{\Psi}_1)\\
& & &= Z_1 + hf(y_1, Z_1) - h\alpha r(y_1, z_1, \Psi_0) + hr(y_1, z_1, \widetilde{\Psi}_1),\\
&(3.8e) \qquad & 0 &= g_y(y_1)v(y_1, z_1),
\end{aligned}
$$

with $\alpha \neq 0$. When $r(y, z, \psi)$ is affine in $\psi$ the 'natural' conjugate symplectic Euler method (3.7) is equivalent to the 'true' conjugate symplectic Euler method (3.8) by considering the relation

$$\widetilde{\Psi}_1 = \alpha\Psi_0 + (1-\alpha)\Psi_1.$$

For (3.6) this corresponds to $\widetilde{\Psi}_1 = \Lambda_0 + \Lambda_1$. Similar to Theorem 3.2 we have:

THEOREM 3.3. *For (3.1), when $r(y, z, \psi)$ is nonlinear in $\psi$, the 'true' conjugate symplectic Euler method (3.8) is consistent of order* 1, *and we have $z_1 - z(t_0 + h) = O(h^2)$. For Hamiltonian systems with holonomic constraints (2.1) the 'true' conjugate symplectic Euler method (3.8) is also symplectic and variational in the sense of Marsden and West.*

**3.4. Global convergence of the symplectic Euler methods.** Since the various symplectic Euler methods are locally independent of the current value of the algebraic variable $\psi$, the errors in the algebraic variables are not propagated. Hence global convergence simply follows from classical results, e.g., [3, Theorem II.3.6 & Theorem III.8.13] since these methods can be expressed as

$$\begin{pmatrix} y_{n+1} \\ z_{n+1} \end{pmatrix} = \begin{pmatrix} y_n \\ z_n \end{pmatrix} + h_n\Phi(t_n, y_n, z_n, h_n).$$

From Theorem 3.2 and Theorem 3.3 we obtain global convergence of order 1 for respectively the 'true' symplectic Euler method (3.5) and the 'true' conjugate symplectic Euler method (3.8). From the proof of Theorem 3.1 it can be seen that the $y$- and $z$-components of the 'natural' symplectic Euler method converge to the exact solution of the inconsistent ODEs

$$
\begin{aligned}
\frac{d}{dt}y &= v(y, z),\\
\frac{d}{dt}z &= f(y, z) + \alpha r(y, z, \Psi_0(y, z)) + (1-\alpha) r(y, z, \Psi_1(y, z))
\end{aligned}
$$

where $\Psi_0(y, z)$ and $\Psi_1(y, z)$ are functions implicitly defined respectively by

$$
\begin{aligned}
0 &= g_y(y)v_z(y, z)(f(y, z) + \alpha r(y, z, \Psi_0)) + \frac{1}{2}g_{yy}(y)(v(y, z), v(y, z)),\\
0 &= \frac{1}{2}g_{yy}(y)(v(y, z), v(y, z)) + g_y(y)v_y(y, z)v(y, z) + (1-\alpha)g_y(y)v_z(y, z)r(y, z, \Psi_1).
\end{aligned}
$$

**4. Numerical experiments.** To illustrate Theorem 3.1 and Theorem 3.2, we have first applied the 'natural' symplectic Euler method (3.2) and the 'true' symplectic Euler method (3.5) with constant stepsize $h$ to the following system

$$\begin{pmatrix} \frac{d}{dt}y_1 \\ \frac{d}{dt}y_2 \end{pmatrix} = \begin{pmatrix} 2z_1 \\ -z_2 \end{pmatrix}, \tag{4.1a}$$

$$\begin{pmatrix} \frac{d}{dt}z_1 \\ \frac{d}{dt}z_2 \end{pmatrix} = \begin{pmatrix} 2y_1y_2z_1z_2 - y_1z_1z_2 \\ z_1 - y_1z_2^3 \end{pmatrix} + \begin{pmatrix} y_2z_1\psi_1^2 \\ -\sqrt{y_1}z_1z_2^2\psi_1 \end{pmatrix}, \tag{4.1b}$$

$$0 = y_1y_2^2 - 1, \tag{4.1c}$$

$$0 = 2y_2(z_1y_2 - y_1z_2). \tag{4.1d}$$

This system of ODAEs is of the form (3.1) with corresponding $r(y, z, \psi)$ being nonlinear in $\psi_1$. This is a purely artificial mathematical test problem. For the initial conditions $y_1(0) = y_2(0) = z_1(0) = z_2(0) = 1$ at $t_0 = 0$ the exact solution to this test problem is given by $y_1(t) = z_1(t) = e^{2t}, y_2(t) = z_2(t) = e^{-t}, \psi_1(t) = e^t$. We have plotted in Fig. 4.1 and Fig. 4.2 the global errors of the 'natural' and 'true' symplectic Euler methods both with parameter $\alpha = 1/2$ for the $y$- and $z$-components at $t_n = 1$ with respect to various constant stepsizes $h$. Logarithmic scales have been used so that a curve appears as a straight line of slope $k$ whenever the leading term of the global error is of order $k$ in the stepsize $h$, i.e., when $\|y_n - y(t_n)\| = O(h^k)$ or $\|z_n - z(t_n)\| = O(h^k)$. For the 'natural' symplectic Euler method we observe

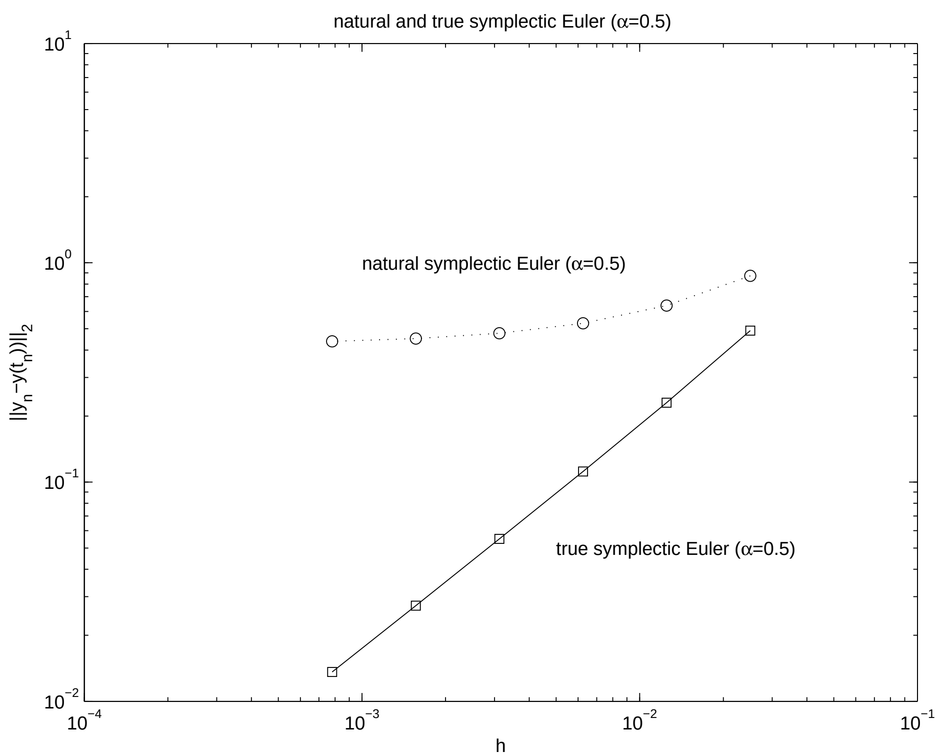


FIG. 4.1. *Global error in $y$ at $t_n = 1$ of the 'natural' and 'true' symplectic Euler methods with parameter $\alpha = 0.5$ applied with various constant stepsizes $h$ to the test problem (4.1).*

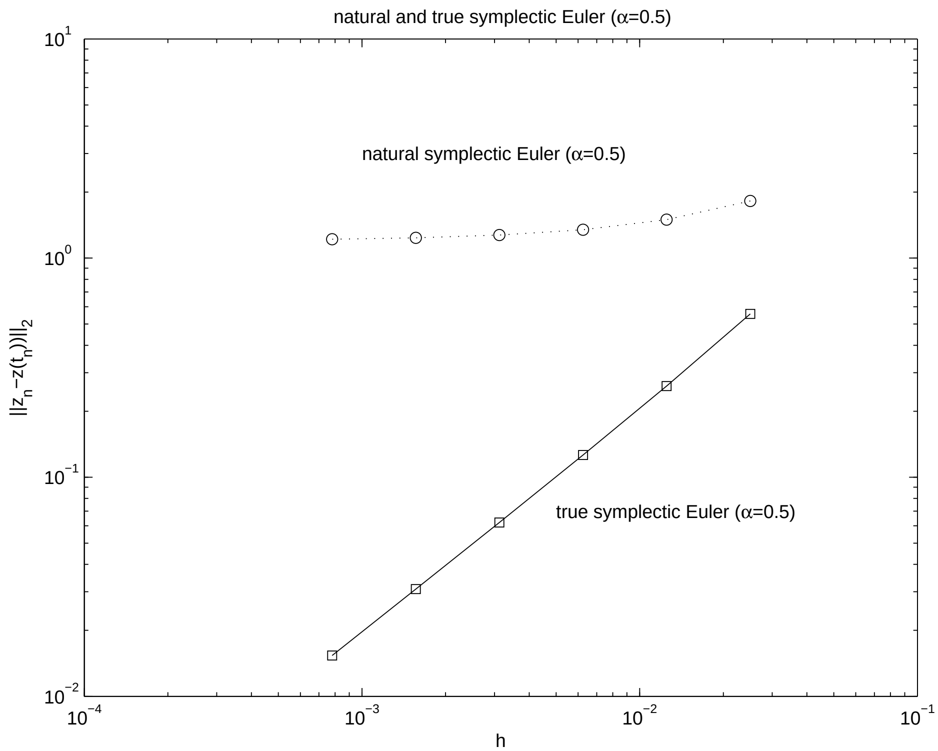


FIG. 4.2. *Global error in $z$ at $t_n = 1$ of the 'natural' and 'true' symplectic Euler methods with parameter $\alpha = 0.5$ applied with various constant stepsizes $h$ to the test problem (4.1).*

the absence of convergence of this method as expected from Theorem 3.1. For the 'true' symplectic Euler method we observe a straight line of slope 1 thus confirming convergence of order 1 as a consequence of Theorem 3.2 and section 3.4.

For the second numerical experiment, we consider a practical model consisting of a mass $m$ subject to gravitation and moving on or possibly above a surface. When the mass is on the surface it is subject to a nonlinear Coulomb friction. The surface that we consider here is a cubic given by

$$x_2 - bx_1^3 = 0$$

where $b$ is a constant. Hence, the position $(y_1, y_2)$ of the mass satisfies $y_2 - by_1^3 \geq 0$. We denote the velocity of the mass by $(z_1, z_2)$. When the mass is on the surface, i.e., $y_2 - by_1^3 = 0$, the constraint is active and we have a system of ODAEs. In this case the normal force $F_N$ due to the reaction of this active holonomic constraint is given by the expression

$$F_N = \begin{pmatrix} -3by_1^2 \\ 1 \end{pmatrix} \psi_1$$

where $\psi_1$ is the Lagrange multiplier associated to the constraint $y_2 - by_1^3 = 0$. The friction force $F_f$ points in the direction opposite to the velocity. If we consider the mass to be in steel and the surface to be in teflon then the norm of the frictional force $\|F_f\|_2$ can be described by the following model of nonlinear Coulomb friction

$\|F_f\|_2 = c_f \|F_N\|_2^{r_f}$ where $c_f \approx 0.1$, $r_f \approx 0.85$, and $\|F_N\|_2$ is the norm of the normal force, see [7, section 10.5]. This nonlinear relation implies that we obtain a system of ODAEs of the form (3.1) which is nonlinear in the Lagrange multiplier $\psi_1$

$$\begin{pmatrix} \frac{d}{dt}y_1 \\ \frac{d}{dt}y_2 \end{pmatrix} = \begin{pmatrix} z_1 \\ z_2 \end{pmatrix}, \tag{4.2a}$$

$$\begin{aligned} m\begin{pmatrix} \frac{d}{dt}z_1 \\ \frac{d}{dt}z_2 \end{pmatrix} &= F_g + F_N + F_f \\ &= \begin{pmatrix} 0 \\ -mg \end{pmatrix} + \begin{pmatrix} -3by_1^2 \\ 1 \end{pmatrix}\psi_1 \\ &\quad -c_f\left((1+9b^2y_1^4)\psi_1^2\right)^{r_f/2}\frac{1}{\sqrt{z_1^2+z_2^2}}\begin{pmatrix} z_1 \\ z_2 \end{pmatrix}, \end{aligned} \tag{4.2b}$$

$$0 = y_2 - by_1^3, \tag{4.2c}$$

$$0 = z_2 - 3by_1^2 z_1. \tag{4.2d}$$

Differentiating (4.2d) with respect to $t$ one can obtain an expression for the exact Lagrange multiplier

$$\psi_1 = \frac{1}{(1+9b^2y_1^4)} m\left(g + 6by_1z_1^2\right)$$

which is clearly independent of the frictional force. Moreover, the matrix corresponding to (3.1e) can also be seen to be independent of the frictional force. When the mass is not on the surface, i.e., when $y_2 - by_1^3 > 0$, the constraint is inactive, and we have a system of ODEs where $\psi_1 = 0$, i.e., $\frac{d}{dt}y = z, m\frac{d}{dt}z = F_g$. The two situations of an active or inactive contraint can be described by the so-called complementarity conditions

$$\psi_1 \cdot (y_2 - by_1^3) = 0, \quad \psi_1 \geq 0, \quad y_2 - by_1^3 \geq 0$$

leading to a system of *overdetermined differential-algebraic inequalities (ODAIs)*. In the numerical experiment given here we will only consider the situation where the constraint is active and that we have a system of ODAEs (4.2). For the constants we have set $m = 1$, $b = 0.01$, $g = 9.81$, $c_f = 0.1$, and $r_f = 0.85$. We consider the following consistent initial conditions at $t_0 = 0$

$$y_1(0) = 10, \quad y_2(0) = 10, \quad z_1(0) = -3.6, \quad z_2(0) = -10.8, \quad \psi_1(0) = 1.7586.$$

We have integrated the system of ODAEs (4.2) up to $t_{end} = 1$. The exact Lagrange multiplier satisfies $\psi_1(t) > 0$ for $t \in [t_0, t_{end}] = [0, 1]$, hence the constraint $0 = y_2 - by_1^3$ remains active. We have plotted in Fig. 4.3 and Fig. 4.4 the global errors of the 'natural' and 'true' symplectic Euler methods both with parameter $\alpha = 1/2$ for the $y$- and $z$-components at $t_n = 1$ with respect to various constant stepsizes $h$. Again logarithmic scales have been used. For the 'natural' symplectic Euler method we observe again the absence of convergence of this method as expected from Theorem 3.1. For the 'true' symplectic Euler method we observe a straight line of slope 1 thus confirming again convergence of order 1 as a consequence of Theorem 3.2 and section 3.4.

**5. Conclusion.** In this paper, we have demonstrated that constrained mechanical systems with force terms that depend nonlinearly on the Lagrange multipliers

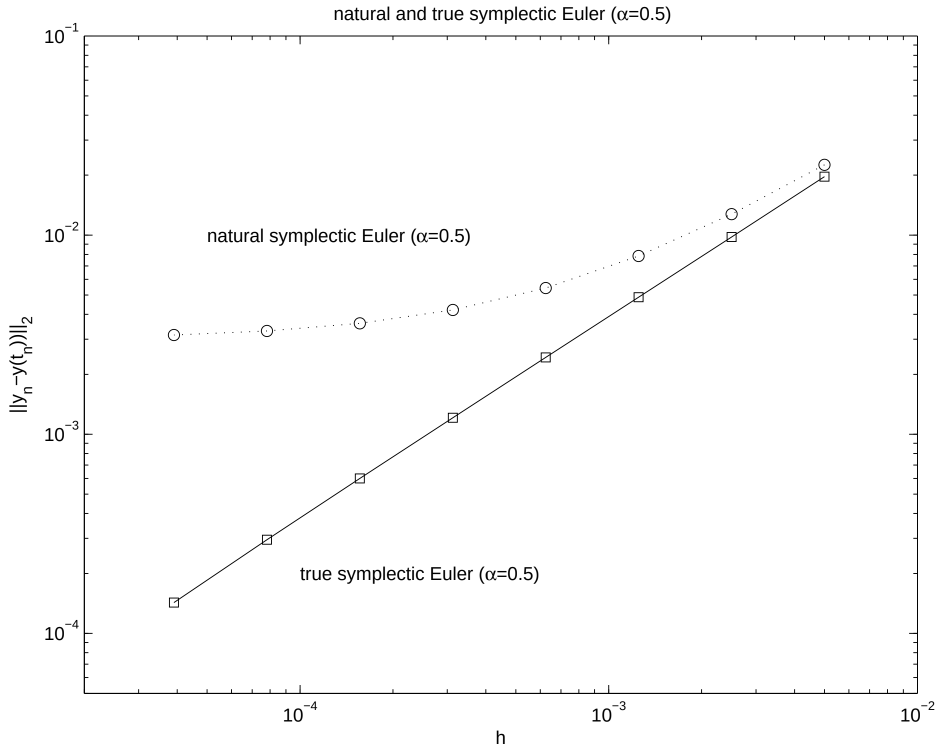


FIG. 4.3. *Global error in $y$ at $t_n = 1$ of the 'natural' and 'true' symplectic Euler methods with parameter $\alpha = 0.5$ applied with various constant stepsizes $h$ to the test problem (4.2).*

require particular care when constructing numerical integration methods. While a straightforward natural extension of the symplectic Euler method fails in this case, the presented 'true' extension is shown to possess the expected convergence order and can be used for the development of higher order methods by composition. This method can be the basis of a time-stepping algorithm for the solution of overdetermined differential-algebraic inequalities (ODAIs) which form an important class of nonsmooth/discontinuous dynamical systems. Though our results are valid for a general class of overdetermined index 2 DAEs, our main focus are systems with friction that arise in both multibody problems where the preservation of nonlinear invariants is of importance.

## REFERENCES


[1] V. Acary and B. Brogliato, *Numerical methods for nonsmooth dynamical systems: applications in mechanics and electronics*, Lect. Notes in Appl. and Comput. Mech., Springer, Berlin, 2008.

[2] E. Hairer, C. Lubich, and G. Wanner, *Geometric numerical integration*, vol. 31 of Comput. Math., Springer, Berlin, 2nd ed., 2006.

[3] E. Hairer, S. P. Nørsett, and G. Wanner, *Solving ordinary differential equations I. Nonstiff problems*, vol. 18 of Comput. Math., Springer, Berlin, 2nd ed., 1993.

[4] E. Hairer and G. Wanner, *Solving ordinary differential equations II. Stiff and differential-algebraic problems*, vol. 14 of Comput. Math., Springer, Berlin, 2nd ed., 1996.

[5] L. O. Jay, *Specialized partitioned additive Runge-Kutta methods for systems of overdetermined*

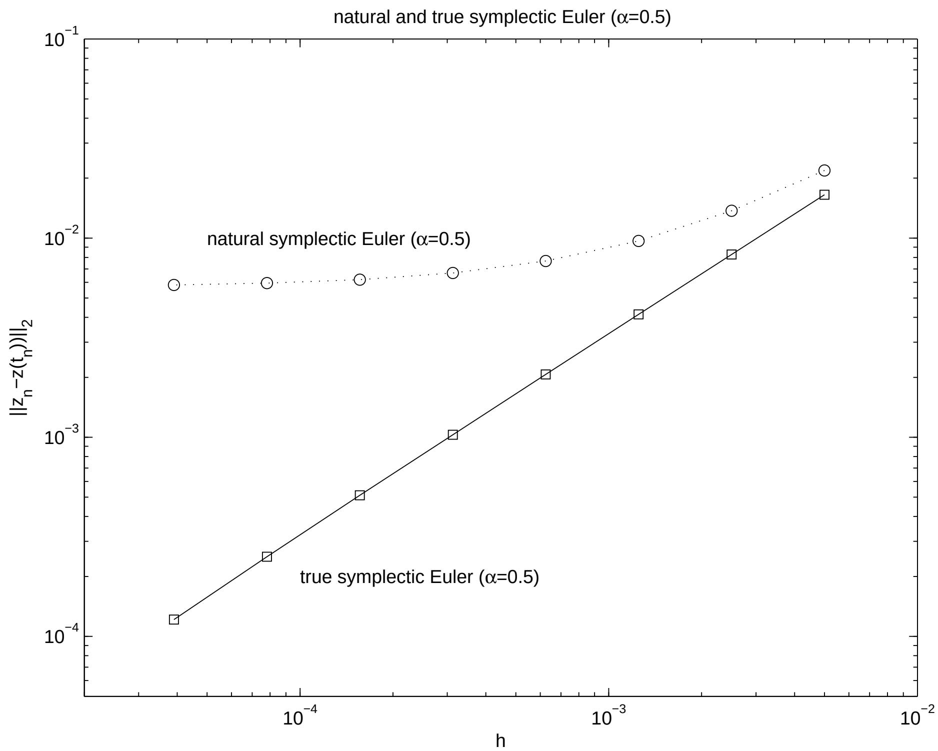


FIG. 4.4. *Global error in* $z$ *at* $t_n = 1$ *of the 'natural' and 'true' symplectic Euler methods with parameter* $\alpha = 0.5$ *applied with various constant stepsizes* $h$ *to the test problem (4.2).*

*DAEs with holonomic constraints*, SIAM J. Numer. Anal., 45 (2007), pp. 1814–1842.
[6] J. E. Marsden and M. West, *Discrete mechanics and variational integrators*, Acta Numerica, (2001), pp. 357–514.
[7] V. L. Popov, *Contact mechanics and friction*, Springer, Berlin, 2010.
[8] S. Reich, *Symplectic integration of constrained Hamiltonian systems by Runge-Kutta methods*, Tech. Report 93-13, Dept. Comput. Sci., Univ. of British Columbia, Canada, 1993.