

Simulation of Constrained Mechanical Systems—Part I: An Equation of Motion

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This paper presents an equation of motion for numerical simulation of constrained mechanical systems with holonomic and nonholonomic constraints. In order to avoid the error accumulation typically experienced in such simulations, the standard equation of motion is enhanced with embedded force and impulse terms which perform continuous constraint and energy correction along the numerical solution. To avoid interference between the kinematic constraint correction and the energy correction terms, both are derived by taking the geometry of the constrained dynamics rigorously into account. In this light, enforcement of the (ideal) holonomic and nonholonomic kinematic constraints are performed using ideal forces and impulses, while the energy conservation law is considered as a nonideal nonlinear nonholonomic constraint on the simulated motion, and as such it is enforced with nonideal forces. As derived, the equation can be directly discretized and integrated with an explicit ODE solver avoiding the need for expensive implicit integration and iterative constraint stabilization. Application of the proposed equation is demonstrated on a representative example. A more elaborate discussion of practical implementation is presented in Part II of this work. [DOI: 10.1115/1.4005572]

1 Introduction

Constrained dynamical systems are traditionally modeled with differential-algebraic equations (DAE), composed of differential equations of the unconstrained motion and a set of algebraic and differential relations which represent kinematic motion constraints. Derivation of such a model is often performed utilizing the Lagrangian equations of the first kind, employing dependent coordinates and algebraic variables (Lagrangian multipliers) which directly incorporate the constraint reaction forces into the equation [1].

The classical method for integration of Lagrangian equations of the first kind is to first represent the kinematic constraints on the acceleration level, then embed these constraints into the equation of motion, and finally integrate the resulting set of ordinary differential equations with a standard ODE solver. As is generally recognized however, direct numerical implementation of this (index-1 DAE problem) ODE formulation (of the original index-3 DAE problem) cannot maintain invariance of the constraint set, which results in motion constraints that drift along the numerical solution, and thus no longer represent the actual dynamics of the system [2].

In addition to the Lagrangian equation of first kind, constrained dynamical systems can also be modeled with approaches developed by Gauss [3], Maggi [4], Gibbs-Appell [5,6], Hamel [7], Kane and Levinson [8], and Udwadia and Kalaba [9–11] as extensively discussed by Pars [12], Neimark and Fufaev [13], Goldstein [14], Arnold [15], Lurie [16], Papastavridis [17], and Vujanović and Atanacković [18]. As generally recognized however, unlike unconstrained systems (modeled with Lagrangian equation of second kind, ODEs, which can be directly discretized and precisely solved with standard ODE solvers), direct utilization of a constrained dynamical model, derived by assuming an *ideal computational environment*, results in error accumulation through numerical simulations. Due to this practical issue, numerical integration of DAEs has attracted considerable research effort, a review of which can be found in [19–24].

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The main question in all DAE problems is, how to ensure that the small numerical error made at each integration step does not accumulate along the solution process. Numerous formulations propose some form of iterative constraint correction on the computed solution to prevent drifting constraints, [25–34,36]. Implementation of such an algorithm often requires a custom built implicit integrator (enhanced with an iterative correction algorithm), development of which may not be trivial [37].

A well-known alternative, which does not utilize iterative correction, was proposed by Baumgarte [38,39]. The approach is motivated with an idea by which artificially added high-gain spring-damper forces can be used to enforce the motion constraints. Although the stiffness-damping constants often require delicate adjustment due to the trade-off between stability and accuracy of the numerical solution, Baumgarte's method is known to be practical; namely, it can be utilized with standard ODE solvers.

Regardless of whether iterative correction is applied or not, it has been recognized that while in many cases the considered DAE is not stiff, the reformulated systems (i.e., Baumgarte's constraint stabilization with highly stiff spring constants chosen to provide precise constraint satisfaction) is stiff by its nature. This specific issue, here related to Baumgarte's method, is also present for many alternative formulations proposed for DAE integration [40]. Practically, this is the reason why integration of constrained dynamical systems (which are originally nonstiff by nature) needs to be performed with a computationally expensive implicit solver usually required to integrate dynamical systems when they are stiff by nature.

Motivated by the research conducted on numerical simulation of constrained dynamical systems, this paper proposes a theoretical development, an *equation of motion* derived for precise long-time simulations with standard explicit ODE solvers. While integration of this equation with an implicit solver is not excluded, the objective here is to focus on explicit integration which is well-suited to real-time simulations [41–43].

Unlike traditional derivations, *the basic assumption during the development of the equation of motion here is that the computational environment is nonideal, the integrated solution is error contaminated, such that, neither the kinematic constraints imposed on the system nor the energy-type conservation law*

considered as an attribute of the system, are exactly satisfied. Using this assumption, a systematic derivation is carried out which results in an equation of motion that directly incorporates the correction terms required for precise satisfaction of the holonomic and nonholonomic kinematic relations and also prevents energy drift along the motion. The separate kinematic constraint correction terms and the energy correction terms are derived to be compatible with each other by taking the geometry of the constrained dynamics rigorously into account. This is achieved by utilizing ideal forces and ideal impulses to correct the simulated motion with respect to the (ideal) kinematic constraints, while using a nonideal constraint force which is tangent to the constraint manifold to enforce an energy type conservation law. This idea, enables *decoupled constraint and energy correction*, which is numerically demonstrated to lead to significant improvement in accuracy over a long time integration.

Compared to the equation presented in [44], the one derived here incorporates nonholonomic constraints and provides a physically consistent means to perform energy conserving DAE integration. These features are recognized as nontrivial to incorporate into many DAE integration methods, which is the main reason why they are rarely offered in the literature. The procedural way to perform this extension of [44] demonstrates the generality of the presented formulation.

The presented equation, which is valid with nonredundant and also redundant constraints, is derived by applying principles of analytical mechanics. However, unlike in classical considerations, Lagrangian multipliers (which are theoretically not defined for redundant constraints [10,21]) have not been utilized. Instead, we employ the Moore-Penrose generalized inverse (pseudoinverse) [45], to represent the explicit equation of constrained motion which regardless of constraint redundancy remains physically consistent [11]. Following derivation, application of the proposed equation is demonstrated on representative examples. Further application on more complex problems together with a discussion of the implementation is provided in Part II of this work.

2 Constrained Dynamical Systems

In this section, the equation of motion for a constrained dynamical system, enhanced with constraint and energy-type correction terms, is presented. The equation derived is fairly general, namely it allows incorporation of holonomic and nonholonomic kinematic constraints, it is valid under redundant constraints and kinematic singularities, and it also provides a *physically consistent* way to perform energy correction along the numerical solution.

2.1 Unconstrained Multibody Dynamics. Consider a dynamical system the configuration of which is uniquely specified by $\mathbf{q} \in \mathbb{R}^n$ generalized coordinates. Let the equation of motion of the considered system be represented in the following form

$$\mathbf{M}(t, \mathbf{q})\ddot{\mathbf{q}} = \mathbf{Q}(t, \mathbf{q}, \dot{\mathbf{q}}) \quad (1)$$

where $\mathbf{M} \in \mathbb{R}^{n \times n}$ is a symmetric and positive definite mass matrix, $\mathbf{Q} \in \mathbb{R}^n$ collects the normal and Coriolis inertial terms and the applied forces. If no constraints are applied on Eq. (1), the dynamical system is considered as unconstrained with respect to the chosen (generalized) coordinates \mathbf{q} .

2.2 Bilateral Constraints: Revised. Let us introduce additional m holonomic and p nonholonomic consistent bilateral constraints on the system dynamics respectively,

$$\Phi_q(t, \mathbf{q}) = \mathbf{0}, \quad \Phi_v(t, \mathbf{q}, \dot{\mathbf{q}}) = \mathbf{0} \quad (2)$$

where $t \in [0, T]$, $\Phi_q: [0, T] \times \mathbb{R}^n \rightarrow \mathbb{R}^m$, $\Phi_v: [0, T] \times \mathbb{R}^{2n} \rightarrow \mathbb{R}^p$. In this section the above constraints will be interpreted as ideal

physical constraints to which the system is subjected. By means of further specification of Eq. (2), we assume that the holonomic constraints are twice differentiable while the nonholonomic constraints are at least once differentiable with respect to all of their respective arguments. In the present context, the intention is to enforce all constraints on the position and velocity levels. In this light, let us redefine Eq. (2) by introducing the extended constraint set as

$$\Phi_q(t, \mathbf{q}) = \mathbf{0}, \quad \dot{\Phi}_q(t, \mathbf{q}, \dot{\mathbf{q}}) = \mathbf{0}, \quad \Phi_v(t, \mathbf{q}, \dot{\mathbf{q}}) = \mathbf{0} \quad (3)$$

The intention here is to replace the nonlinear position and velocity level constraints Eq. (3) with two separate constraint sets, one which is linear with respect to velocities and another which is linear with respect to the accelerations. In this light, let us denote the holonomic constraints that evolve along the dynamic trajectory with $\Phi_q(t) := \Phi_q(t, \mathbf{q}(t))$, and define a first order Taylor expansion of this function as,

$$\Phi_q(t + dt) = \Phi_q(t) + (\mathbf{A}_q \dot{\mathbf{q}} - \mathbf{b}_q)dt + O(dt^2)$$

where $\mathbf{A}_q(t, \mathbf{q}) = \partial\Phi_q/\partial\mathbf{q}$ and $\mathbf{b}_q(t, \mathbf{q}) = -\partial\Phi_q/\partial t$. Similarly, one can define the Taylor expansion for $\dot{\Phi}_q(t) := \dot{\Phi}_q(t, \mathbf{q}(t), \dot{\mathbf{q}}(t))$ and $\Phi_v(t) := \Phi_v(t, \mathbf{q}(t), \dot{\mathbf{q}}(t))$ respectively as,

$$\dot{\Phi}_q(t + dt) = \dot{\Phi}_q(t) + (\mathbf{A}_q \ddot{\mathbf{q}} - \mathbf{b}_{qv})dt + O(dt^2)$$

where $\mathbf{b}_{qv}(t, \mathbf{q}, \dot{\mathbf{q}}) = -(\partial((\partial\Phi_q/\partial\mathbf{q})\dot{\mathbf{q}})/\partial\mathbf{q})\dot{\mathbf{q}} - 2(\partial^2\Phi_q/\partial t\partial\mathbf{q})\dot{\mathbf{q}} - \partial^2\Phi_q/\partial t^2$ and

$$\Phi_v(t + dt) = \Phi_v(t) + (\mathbf{A}_v \ddot{\mathbf{q}} - \mathbf{b}_{vv})dt + O(dt^2)$$

where $\mathbf{A}_v(t, \mathbf{q}, \dot{\mathbf{q}}) = \partial\Phi_v/\partial\dot{\mathbf{q}}$ and $\mathbf{b}_{vv}(t, \mathbf{q}, \dot{\mathbf{q}}) = -(\partial\Phi_v/\partial\mathbf{q})\dot{\mathbf{q}} - \partial\Phi_v/\partial t$. If dt is interpreted as a small numerical integration step, then by utilizing $\Phi_q(t + dt) = \mathbf{0}$, $\dot{\Phi}_q(t + dt) = \mathbf{0}$, and $\Phi_v(t + dt) = \mathbf{0}$, the first order approximation of Eq. (3) can be satisfied with constraints defined by

$$\mathbf{A}_q \dot{\mathbf{q}} = \mathbf{b}_q - \Delta_q \quad (4)$$

$$\mathbf{A}_v \ddot{\mathbf{q}} = \mathbf{b}_v - \Delta_v \quad (5)$$

where $\mathbf{A}_v = (\mathbf{A}_q^T, \mathbf{A}_{vv}^T)^T$, $\mathbf{b}_v = (\mathbf{b}_{qv}^T, \mathbf{b}_{vv}^T)^T$ while $\Delta_q = \Phi_q/dt$ and $\Delta_v = (\dot{\Phi}_q^T/dt, \Phi_v^T/dt)^T$.

In contrast to many traditional velocity and acceleration level constraint representations, the one presented above does not assume an ideal, error-free computational environment or constraint consistent initial conditions. Practically, Eqs. (4) and (5) incorporate the position $\Phi_q \approx \mathbf{0}$ and also velocity level error $\dot{\Phi}_q \approx \mathbf{0}$, $\Phi_v \approx \mathbf{0}$ (expected) along the numerical integration. Note that, if the constraints are all holonomic, then $\mathbf{A}_q = \mathbf{A}_v$ and $\Delta_v = \dot{\Phi}_q/dt$, such that Eqs. (4) and (5) would reduce to the form presented in Ref. [44]. On the other hand, in an ideal computational environment, Eq. (4) would be identically satisfied while Eq. (5) would reduce to the standard acceleration level constraints: $\mathbf{A}_v \ddot{\mathbf{q}} = \mathbf{b}_v$.

2.3 Orthogonal Decomposition of the Constraint Reactions. Let us now assign a generalized constraint force \mathbf{Q}_c and a generalized constraint impulse \mathbf{I}_c to the acceleration and velocity level kinematic constraints, respectively. Note that while the (smooth) bilateral constraints (considered in this paper) only produce a constraint force, we will also introduce \mathbf{I}_c to eliminate the error that is *independently* induced on the velocity level at each integration step.

In the following, we introduce a dynamically consistent orthogonal decomposition of the generalised impulses and forces with respect to the constraint manifold,

$$\mathbf{I}_c = \mathbf{I}_{c\perp} + \mathbf{I}_{c\parallel} = \mathbf{R}^T \mathbf{T}_q \mathbf{R}^{-T} \mathbf{I}_c + \mathbf{R}^T \mathbf{N}_q \mathbf{R}^{-T} \mathbf{I}_c \quad (6)$$

and

$$\mathbf{Q}_c = \mathbf{Q}_{c\perp} + \mathbf{Q}_{c\parallel} = \mathbf{R}^T \mathbf{T}_v \mathbf{R}^{-T} \mathbf{Q}_c + \mathbf{R}^T \mathbf{N}_v \mathbf{R}^{-T} \mathbf{Q}_c \quad (7)$$

where $\mathbf{T}_* = \mathbf{C}_*^+ \mathbf{C}_*$, $\mathbf{N}_* = \mathbf{I} - \mathbf{C}_*^+ \mathbf{C}_*$ ($\mathbf{I} \in \mathbb{R}^{n \times n}$ is an identity matrix) are orthogonal projection operators defined for $q/v = (*)$, where $\mathbf{C}_* = \mathbf{A}_* \mathbf{R}^{-1}$ is the constraint matrix weighted with an upper triangular Cholesky factor of the mass matrix $\mathbf{M} = \mathbf{R}^T \mathbf{R}$ while \mathbf{C}_*^+ is the (Moore-Penrose generalized inverse) pseudoinverse of \mathbf{C}_* [45]. Note that this orthogonal decomposition is consistent with the one proposed in Ref. [46].

According to the D'Alembert principle, a constraint force is ideal if it is orthogonal to the (acceleration level) constraint manifold [47]. In this light, if the constraint force is assumed to be ideal, it implies $\mathbf{Q}_c = \mathbf{Q}_{c\perp}$. On the other hand, $\mathbf{Q}_c = \mathbf{Q}_{c\perp} + \mathbf{Q}_{c\parallel}$, where $\mathbf{Q}_{c\parallel}$ is attributed as a nonideal constraint force component which is tangent to the constraint manifold [11,48]. Following the same geometrical interpretation, one can analogously introduce an ideal constraint impulse $\mathbf{I}_{c\perp}$ which is normal to the (velocity) constraint manifold and the corresponding nonideal impulse component $\mathbf{I}_{c\parallel}$ which lies in the respective tangential direction.

It is important to point out that in the present paper we consider *ideal kinematic constraints*, such that the nonideal force component introduced above is not used to model general nonideal constraint forces, but will only be used to develop a physically consistent energy conserving integration, see Sec. 2.5. Practically, while nonideal constraint forces are not excluded here, it would be more precise to interpret and incorporate such (constraint) forces as applied forces, see Refs. [17,49,50], rather than consider them as "tangent" components of the constraint reaction forces.

2.4 Constrained Multibody Dynamics. In this section we will incorporate the position and velocity-level constraints into the dynamic equations. In particular, the presented derivation employs generalized inverse theory to derive a constraint force and the explicit equation of the constrained motion.

Let us start with a general representation of the constrained dynamical system,

$$\mathbf{M} \ddot{\mathbf{q}} = \mathbf{Q} + \mathbf{Q}_c \quad (8)$$

where \mathbf{Q}_c is the generalized constraint force. In order to derive \mathbf{Q}_c in explicit form, the constrained acceleration is first defined from Eq. (8), then the result is substituted back to the acceleration level constraints Eq. (5), to obtain a linear equation

$$\mathbf{A}_v \mathbf{M}^{-1} \mathbf{Q}_c = \mathbf{b}_v - \mathbf{A}_v \mathbf{a} - \Delta_v \quad (9)$$

where $\mathbf{a} = \mathbf{M}^{-1} \mathbf{Q}$ is the unconstrained acceleration that the system would have without the imposed constraints, see Eq. (1). As a next preparation step, we will define, $\mathbf{C}_v = \mathbf{A}_v \mathbf{R}^{-1}$, and $\mathbf{M}^{-1} = \mathbf{R}^{-1} \mathbf{R}^{-T}$ using the upper triangular Cholesky factor of the mass-matrix \mathbf{R} . By utilizing these two relations, the above linear equation becomes,

$$\mathbf{C}_v \mathbf{R}^{-T} \mathbf{Q}_c = \mathbf{b}_v - \mathbf{A}_v \mathbf{a} - \Delta_v \quad (10)$$

If the constraint force is assumed ideal $\mathbf{Q}_c = \mathbf{Q}_{c\perp}$, one could define it through a pseudoinverse solution of Eq. (9), that provides, $\mathbf{Q}_c^T \mathbf{M}^{-1} \mathbf{Q}_c \rightarrow \min$. However, to incorporate the possibly nonideal force component, we will recall a general solution of Eq. (10) defined below,

$$\begin{aligned} \mathbf{Q}_c &= \mathbf{Q}_{c\perp} + \mathbf{Q}_{c\parallel} \\ &= \mathbf{R}^T \mathbf{C}_v^+ (\mathbf{b}_v - \mathbf{A}_v \mathbf{a} - \Delta_v) + \mathbf{R}^T \mathbf{N}_v \mathbf{R}^{-T} \mathbf{Q}_0 \end{aligned} \quad (11)$$

In the obtained relation, the ideal constraint forces $\mathbf{Q}_{c\perp}$ (which act normal to the constraint manifold) are explicitly defined by the imposed kinematic constraints Eq. (5). On the other hand, one would need additional physical information regarding \mathbf{Q}_c in order to specify \mathbf{Q}_0 and as such $\mathbf{Q}_{c\parallel} = \mathbf{R}^T \mathbf{N}_v \mathbf{R}^{-T} \mathbf{Q}_0$. In contrast to traditional simulation approaches, where by means of the D'Alembert principle, the nonideal force component is neglected, we will show, in Sec. 2.5, that this component can be used to prevent error accumulation on the constraint consistent motion.

In order to proceed further, let us define the constrained acceleration, $\dot{\mathbf{q}} = \dot{\mathbf{v}}$, substitute Eq. (11) into Eq. (8) and rewrite the resulting equation in the following first order form

$$\dot{\mathbf{q}} = \mathbf{v} \quad (12)$$

$$\dot{\mathbf{v}} = \mathbf{a} + \mathbf{R}^{-1} \mathbf{C}_v^+ (\mathbf{b}_v - \mathbf{A}_v \mathbf{a} - \Delta_v) + \mathbf{R}^{-1} \mathbf{N}_v \mathbf{R}^{-T} \mathbf{Q}_0 \quad (13)$$

Although this formulation incorporates the numerical errors at the velocity level, $\dot{\Phi}_q \approx \mathbf{0}$ and $\Phi_v \approx \mathbf{0}$, it cannot in general prevent error accumulation. This is because Eqs. (12) and (13) do not yet take the numerically induced position level error, given by $\Phi_q \approx \mathbf{0}$, into account. Due to this reason, we introduce an additional correction term in the velocity equation by adding a generalized impulse to Eq. (12) as

$$\dot{\mathbf{q}} = \mathbf{v} + \mathbf{M}^{-1} \mathbf{I}_c \quad (14)$$

This impulse, \mathbf{I}_c , is not generated by the constraints but rather is introduced to compensate for numerical errors that are independently induced on velocity level along the integration. A similar velocity level constraint correction was used in Refs. [21,26,41]. By substituting Eq. (14) into Eqs. (4) and utilizing the same solution procedure used to solve (10), the compensation term becomes

$$\begin{aligned} \mathbf{I}_c &= \mathbf{I}_{c\perp} + \mathbf{I}_{c\parallel} \\ &= \mathbf{R}^T \mathbf{C}_q^+ (\mathbf{b}_q - \mathbf{A}_q \mathbf{v} - \Delta_q) + \mathbf{R}^T \mathbf{N}_q \mathbf{R}^{-T} \mathbf{I}_0 \end{aligned} \quad (15)$$

Note that similar to the constraint force, \mathbf{I}_c is separated into an ideal impulse (first term), which is normal to the velocity constraint manifold, and a nonideal impulse (second term), which is tangent to the constraint manifold. Substituting Eq. (15) into Eq. (14), and considering the obtained relation together with Eq. (13), the complete equation of motion for the constrained dynamical system is obtained

$$\dot{\mathbf{q}} = \mathbf{v} + \mathbf{R}^{-1} \mathbf{C}_q^+ (\mathbf{b}_q - \mathbf{A}_q \mathbf{v} - \Delta_q) \quad (16)$$

$$\dot{\mathbf{v}} = \mathbf{a} + \mathbf{R}^{-1} \mathbf{C}_v^+ (\mathbf{b}_v - \mathbf{A}_v \mathbf{a} - \Delta_v) + \mathbf{R}^{-1} \mathbf{N}_v \mathbf{R}^{-T} \mathbf{Q}_0 \quad (17)$$

where \mathbf{a} is the unconstrained acceleration, $\dot{\mathbf{v}}$ is the corrected constrained acceleration, $\dot{\mathbf{q}}$ is the corrected constrained velocity, while specification of \mathbf{Q}_0 is the subject of the following discussion. The present formulation utilizes the Cholesky factorization of the mass matrix instead of relying on its principal square root $\mathbf{M}^{1/2}$ used by Udawadia and Kalaba [11]. Regardless of this difference, equivalence between the above equation and the one proposed in Ref. [11] in an ideal computational environment is provided.²

Since the smooth holonomic constraint enforcement is fully addressed with the ideal impulse term, we have used $\mathbf{I}_0 = \mathbf{0}$ in the derivation of Eq. (16). By recalling D'Alembert's principle, Eq.

²In an ideal computational environment, the constraints would be exactly satisfied, which would result in, $\Delta_q = \mathbf{0}$, $\Delta_v = \mathbf{0}$, and $\mathbf{A}_q \mathbf{v} = \mathbf{b}_q$. In that case, $\dot{\mathbf{q}} = \mathbf{v}$, and Eq. (17) would reduce to $\ddot{\mathbf{q}} = \mathbf{a} + \mathbf{R}^{-1} \mathbf{C}_v^+ (\mathbf{b}_v - \mathbf{A}_v \mathbf{a}) + \mathbf{R}^{-1} \mathbf{N}_v \mathbf{R}^{-T} \mathbf{Q}_0$. The last two terms in this equation originate from the general solution of the linear Eq. (10). The same general solution obtained from a linear Eq. (9) would result in $\dot{\mathbf{q}} = \mathbf{a} + \mathbf{M}^{-1/2} \mathbf{B}^+ (\mathbf{b}_v - \mathbf{A}_v \mathbf{a}) + \mathbf{M}^{-1/2} (\mathbf{I} - \mathbf{B}^+ \mathbf{B}) \mathbf{M}^{-1/2} \mathbf{Q}_0$, where $\mathbf{M} = \mathbf{M}^{1/2} \mathbf{M}^{1/2}$ and $\mathbf{B} = \mathbf{A}_v \mathbf{M}^{-1/2}$. This equation is the one proposed by Udawadia and Kalaba [11].

(17) could also be simplified by assuming that the constraint reaction force is ideal, $\mathbf{Q}_0 = \mathbf{0}$. By utilizing this assumption and restricting the constraints to be holonomic, in which case $\mathbf{A}_v = \mathbf{A}_q$ ($\mathbf{C}_v = \mathbf{C}_q$), the above equation reduces to the one proposed by the authors [44]. However, the force component related to \mathbf{Q}_0 can be interpreted as a nonideal reaction force which can only alter the motion of the system on the constrained manifold. Accordingly, this constraint force is a natural candidate to eliminate numerically induced energy dissipation (or addition). With emphasis on this idea we will further discuss how to define \mathbf{Q}_0 .

2.5 Generalized Energy Correction with Nonideal Constraint Forces. Let us now assume that, for the considered mechanical system, one is able to find a generalized energy-type conservation law (that is a nonlinear functions of time, position and velocity) defined by

$$\Phi_e(t, \mathbf{q}, \dot{\mathbf{q}}) = E(t, \mathbf{q}, \dot{\mathbf{q}}) - E_0 - \int_0^t \dot{E} d\tau = 0 \quad (18)$$

where $\Phi_e : [0, T] \times \mathbb{R}^{2n} \rightarrow \mathbb{R}$ is the energy conservation law, $E : [0, T] \times \mathbb{R}^{2n} \rightarrow \mathbb{R}$ represents the total mechanical energy of the system, E_0 is the energy of the system at initialization, while \dot{E} is the energy input rate to the system (for conservative systems $\dot{E} \equiv 0$). While Φ_e is interpreted here as an energy-type conservation law [34], it can, without restriction on generality, represent a nonenergy type conserved quantity as well [51]. Note that under ideal integration, the conservation law Eq. (18) would be exactly satisfied along the solution, indicating that Eq. (18) is different by nature than the kinematic constraints imposed on the motion [17]. Numerical integrations however are never ideal, and as such Eq. (18) is not expected to be satisfied automatically.

There are two general ways to enforce Eq. (18) along the numerical solution. One can either embed the energy relation in the *ideal* nonholonomic constraint set [34,52], in which case Eq. (18) would be enforced with ideal constraint forces, or one can utilize a specific implicit discretization scheme [32,53], which provides automatic energy conservation. Instead of adapting one of these approaches, we consider the energy relation as a *nonideal nonlinear nonholonomic constraint* during the error contaminated simulation. This idea allows us to perform physically consistent energy correction by following the procedure used in Sec. 2.4 for kinematic constraint enforcement. In this light, let us first represent the energy relation on an acceleration level as,

$$\mathbf{A}_e \ddot{\mathbf{q}} = b_e - \Delta_e \quad (19)$$

where $\mathbf{A}_e(t, \mathbf{q}, \dot{\mathbf{q}}) = \partial \Phi_e / \partial \dot{\mathbf{q}}$, $b_e(t, \mathbf{q}, \dot{\mathbf{q}}) = -\partial \Phi_e / \partial t - (\partial \Phi_e / \partial \mathbf{q}) \dot{\mathbf{q}}$ and $\Delta_e = \Phi_e / dt$. One can now calculate \mathbf{Q}_0 in order to maintain Eq. (19). For this purpose, let us first replace the ideal constrained acceleration $\ddot{\mathbf{q}}$ in Eq. (19) with its corrected counterpart $\ddot{\mathbf{v}}$ defined by Eq. (17), and then solve the corresponding equation to obtain

$$\mathbf{Q}_0 = \mathbf{R}^T [\mathbf{C}_e \mathbf{N}_v]^+ (b_{ev} - \mathbf{A}_{ev} \mathbf{a} - \Delta_{ev}) \quad (20)$$

where $\mathbf{C}_e = \mathbf{A}_e \mathbf{R}^{-1}$ and $(*)_{ev} = (*)_e - \mathbf{C}_e \mathbf{C}_v^+ (*)_v$. This force, \mathbf{Q}_0 , is specifically chosen to provide $\mathbf{Q}_0^T \mathbf{M}^{-1} \mathbf{Q}_0 \rightarrow \min$. Substituting Eq. (20) into Eq. (17), one obtains the equation of motion enhanced with a *nonideal energy correction force*.³ In principle, nonlinearly nonholonomic kinematic constraints are rare in

³In an ideal computational environment, the kinematic constraints and the energy law would be exactly satisfied, (i.e., $\Delta_{ev} = 0$), and thus the constrained acceleration could be exactly computed $\ddot{\mathbf{q}} = \mathbf{a} + \mathbf{R}^{-1} \mathbf{C}_v^+ (b_v - \mathbf{A}_v \mathbf{a})$. In that case, Eq. (20) would reduce to $\mathbf{Q}_0 = \mathbf{R}^T [\mathbf{C}_e \mathbf{N}_v]^+ \mathbf{A}_e (\ddot{\mathbf{q}} - \mathbf{a} - \mathbf{R}^{-1} \mathbf{C}_v^+ (b_v - \mathbf{A}_v \mathbf{a}))$, and as such it would not perform any correction, $\mathbf{Q}_0 = \mathbf{0}$.

practice [13,54], and as such they are usually not considered in multibody simulations. However, incorporation of these constraints as described here is recognized as a natural and physically interpretable way to perform a generalized energy type correction.

In summary, the overall correction effort proposed in this paper has two dynamically independent parts; one is the constraint correction while another is the energy correction. The kinematic constraint correction is performed with ideal generalized forces and impulses which act orthogonal to the constraint manifold (and as such can neither add nor dissipate energy from the system) [44]. On the other hand the energy correction is performed with a nonideal force component, $\mathbf{R}^T \mathbf{N}_v \mathbf{R}^{-T} \mathbf{Q}_0$, which can actively inject or dissipate energy during the numerical simulation in order to maintain Eq. (18). As derived, the nonideal correction can only alter the motion which is consistent with the (ideal) kinematic constraints and as such it cannot interfere with the terms used for the kinematic constraint enforcement. We refer to this energy correction as *physically consistent*, which, as demonstrated in Sec. 4, can lead to a significant accuracy improvement in numerical integration.

3 Comments on the Proposed Equation

The original formulation of the considered constrained dynamical problem Eqs. (1) and (2) is an index-3 differential algebraic equation [2], which requires special numerical algorithms for its precise integration. On the other hand, the present equation can be directly discretized using explicit ODE schemes (Forward Euler, Runge-Kutta, etc.) and integrated in the same fashion as one would integrate ordinary differential equations. This implementational convenience, which is also the main advantage of Baumgarte's method, is of high practical importance. Beyond this, the presented formulation offers an added benefit. Indeed, while Baumgarte's formulation becomes stiff when precise constraint enforcement is required (i.e., highly stiff springs should be used to precisely enforce the kinematic constraints), an accurate integration with Eqs. (16), (17), and (20) does not lead to stiff formulation. This is because the terms containing, $1/dt$, that could lead to a stiff formulation when the step size is reduced, will be canceled out once an explicit discretization is applied (see the discretized equations in Part II of this work).

While the *constraint accuracy* (i.e., accuracy measured on the constraints) is frequently used to characterize the precision of a DAE solution, this error indicator may not fully characterize the accuracy of the considered numerical solution. Namely along the integration, the constraints can be precisely satisfied (using

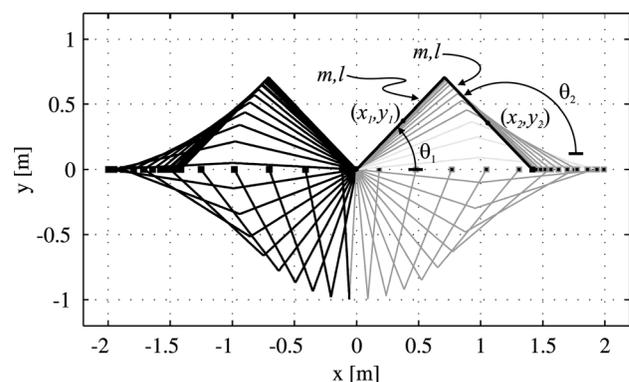


Fig. 1 Slider-crank mechanism: $l = 1$ m, $m = 1$ kg. The simulation is performed for $t \in [0, 100]$ s started from $\mathbf{q}(0) = [\sqrt{2}/4, \sqrt{2}/4, \pi/4, 3\sqrt{2}/4, \sqrt{2}/4, -\pi/4]^T$, $\mathbf{v}(0) = [0, 0, 0, 0, 0, 0]^T$ and conducted with 5×10^{-2} s time step. The stroboscopic view represents the motion for $t \in [96.9, 99]$ s.

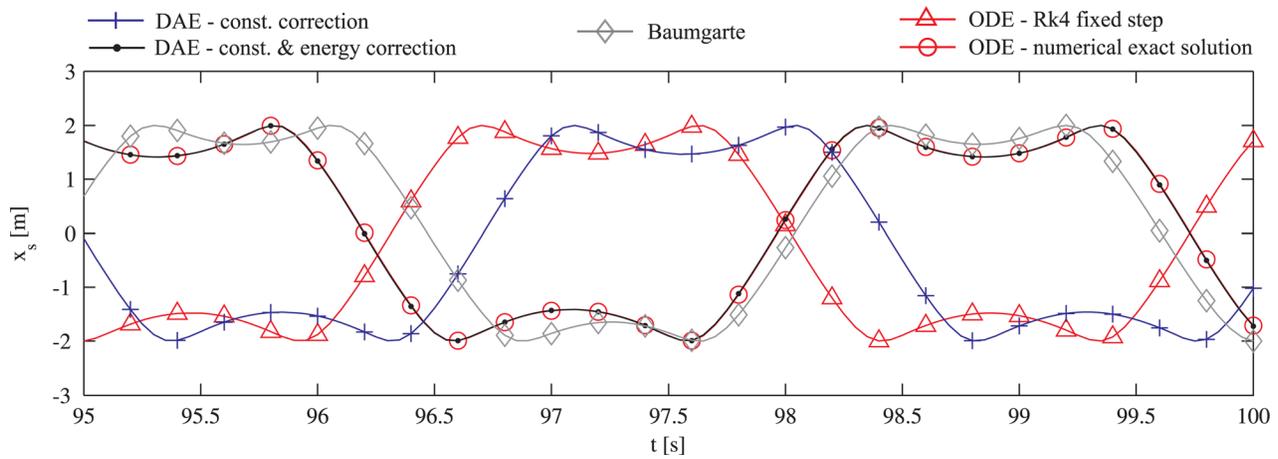


Fig. 2 Horizontal motion of the slider, $x_s = x_2 + (l/2)\cos(\theta_2)$ vs time. The picture shows that the solution obtained with the proposed DAE integration method (with 5×10^{-2} s time step) is well matched with the numerically exact ODE solution.

iterative corrections up to round-off errors after each time step), while the response of the system may, for example, be delayed in time with respect to the *exact solution*. This kind of error accumulation (also present during ODE integration) is inevitable in numerical simulations. Using the proposed energy correction scheme however, one can reduce (although not eliminate) the error that accumulates along the constraint consistent motion. Indeed, it is subsequently demonstrated (and also shown in Part II of this work) that the combined kinematic constraint correction and kinetic energy correction can lead to more precise solutions.

Finally, let us point out that pseudo-inversion is a convenient *theoretical tool* utilized to present a general formulation,

Eqs. (16), (17), and (20), which is valid even in the case of constraint redundancy and kinematic singularities [35]. Due to its generality, direct implementation of this formulation may be computationally expensive. Note however that in practice, Eqs. (16), (17), and (20) can be implemented without forming the pseudo-inverses explicitly. Moreover, if the constraints are nonredundant (as is usually assumed in literature) pseudo-inversion is not required, and one can implement the proposed equation using the same linear algebra routines used to implement many other DAE equation. In Part II of this work [55], we specifically discuss a MATLAB/SIMULINK implementation of the developed equation which was used to perform real-time multibody simulations.

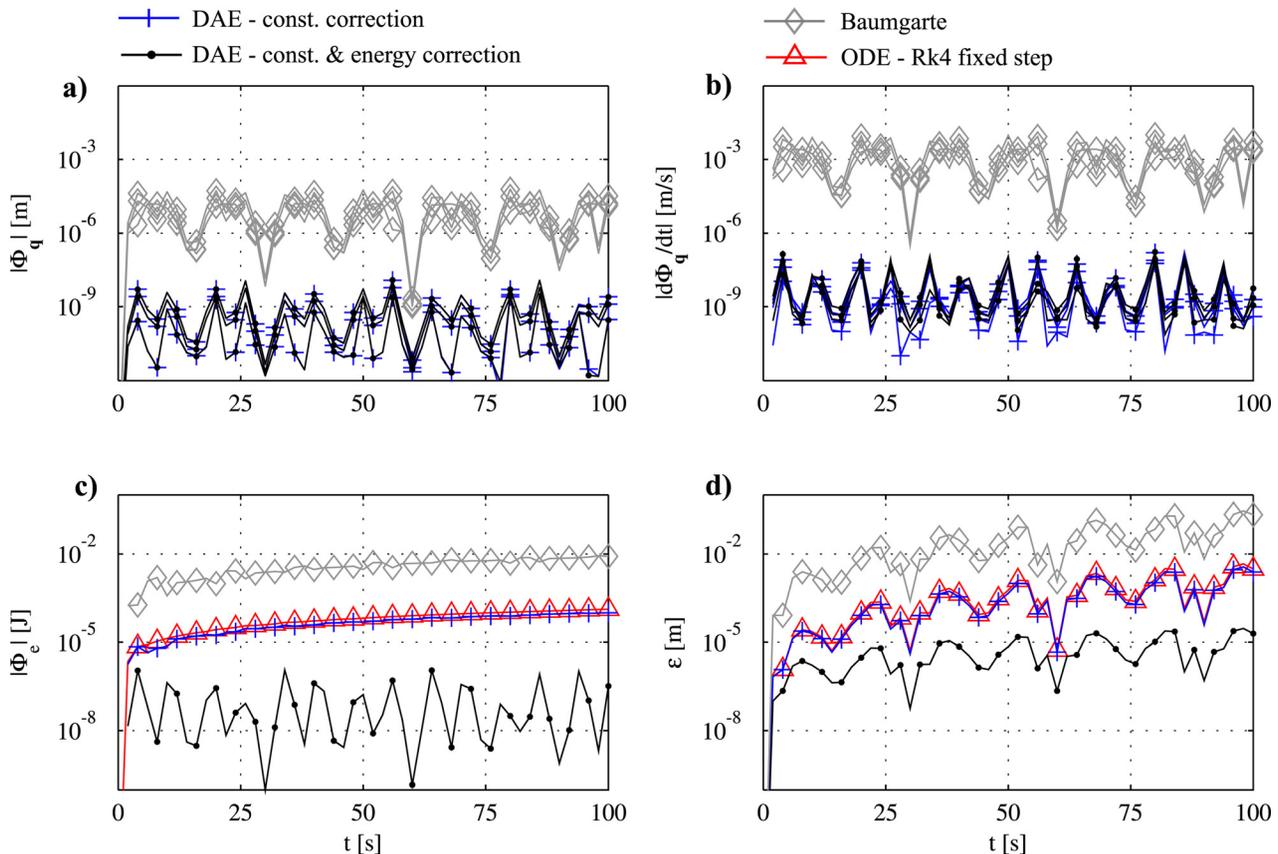


Fig. 3 From top to bottom the semilog pictures depict: $|\Phi_q|$, $|\dot{\Phi}_q|$, $|\Phi_e|$, and $\epsilon = \sqrt{dx^2 + dy^2}$, where dx and dy are measured with respect to the numerically exact ODE solution. The integration here is performed with 10^{-2} s time step.

4 Application

Using the proposed equation of motion, Eqs. (16), (17), and (20), representative simulations are presented. The test examples chosen in this paper allow derivation of an unconstrained model, which when solved with a variable step `MATLAB` solver (`ode45(*)`) with 10^{-12} relative and 10^{-12} absolute tolerance provide a *numerically exact solution*.⁴ This solution is an ideal reference which allows us to deduce the *overall accuracy* of the proposed DAE solution obtained with Eqs. (16), (17), and (20). The accuracy of the proposed DAE integrator is also assessed by reporting the *constraint accuracy*,⁵ and the *energy accuracy*⁶ of the obtained solutions. For further comparison, we also provide a DAE reference solution obtained using Baumgarte's constrained stabilization (implemented with optimal parameters [42]). In order to assess the proposed formulation, long time simulations are presented. The examples are solved with a fourth order fixed step Runge-Kutta (RK4) method implemented in `MATLAB`. The implementation details are described in Part II of this work. All physical quantities used in the simulations have standard SI units [kg, m, s], while $g = 9.81 \text{ m/s}^2$.

4.1 Slider-Crank Mechanism. The slider-crank mechanism consisting of two links with equal lengths l and masses m is shown in Fig. 1. By means of constrained dynamics, there are many different formulations which can be used to simulate the motion of this system. In this paper, we utilize six absolute coordinates $\mathbf{q} = [x_1, y_1, \theta_1, x_2, y_2, \theta_2]^T$. With this coordinate choice, the unconstrained equation $\mathbf{M}\ddot{\mathbf{q}} = \mathbf{Q}$ is given in the following simple form

$$\begin{bmatrix} m & 0 & 0 & 0 & 0 & 0 \\ 0 & m & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{12}ml^2 & 0 & 0 & 0 \\ 0 & 0 & 0 & m & 0 & 0 \\ 0 & 0 & 0 & 0 & m & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{12}ml^2 \end{bmatrix} \begin{bmatrix} \ddot{x}_1 \\ \ddot{y}_1 \\ \ddot{\theta}_1 \\ \ddot{x}_2 \\ \ddot{y}_2 \\ \ddot{\theta}_2 \end{bmatrix} = \begin{bmatrix} 0 \\ -mg \\ 0 \\ 0 \\ -mg \\ 0 \end{bmatrix} \quad (21)$$

where the mass matrix is constant and diagonal. To model the slider-crank mechanism as a constrained dynamical system, Eq. (21) is subjected to five holonomic constraints

$$\Phi_{\mathbf{q}} = \begin{bmatrix} x_1 - (l/2)\cos(\theta_1) \\ y_1 - (l/2)\sin(\theta_1) \\ x_1 + (l/2)\cos(\theta_1) - x_2 + (l/2)\cos(\theta_2) \\ y_1 + (l/2)\sin(\theta_1) - y_2 + (l/2)\sin(\theta_2) \\ y_2 + (l/2)\sin(\theta_2) \end{bmatrix} = \mathbf{0} \quad (22)$$

where (x_1, y_1) and (x_2, y_2) are coordinates of the center of mass of the links, while θ_1 and θ_2 are absolute link angles measured counterclockwise from a horizontal reference. Beyond the kinematic constraints, an energy conservation law,

$$\Phi_e = \frac{1}{2}\dot{\mathbf{q}}^T \mathbf{M}\dot{\mathbf{q}} + mgy_1 + mgy_2 - E_0 = 0 \quad (23)$$

is incorporated as a nonideal nonlinear nonholonomic constraint on the numerical integration.

⁴The numerically exact solution is an *ideal reference* along which the constraints are *exactly* satisfied.

⁵The constraint accuracy is reported by depicting the error on the kinematic constraints.

⁶The energy accuracy is reported by depicting the energy error.

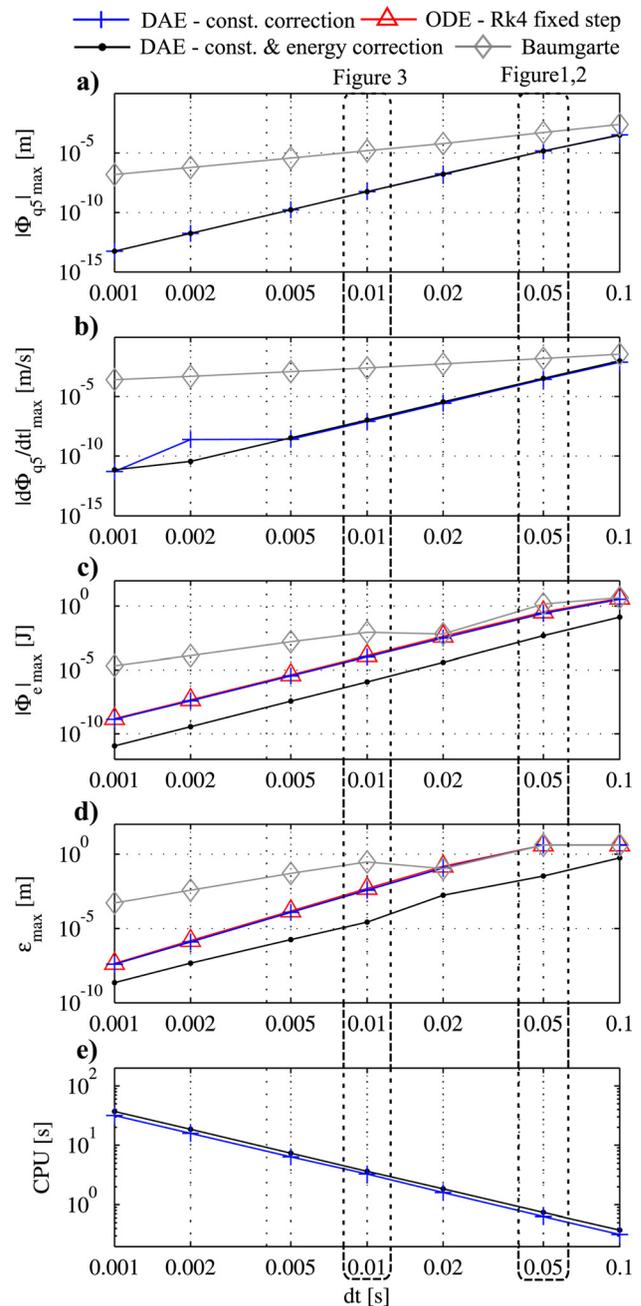


Fig. 4 From top to bottom the log-log pictures depict the maximum constraint error, the maximum energy error and the maximum overall error. The accuracy/step-size characterizations are performed through a $t \in [0, 100]$ s simulation. On the last plot, the CPU time corresponding to integration with and without energy correction is presented.

Figure 1 shows a stroboscopic view of the motion obtained with large time step (i.e., 5×10^{-2}), using the proposed DAE integration method. The corresponding motion of the sliding end of the mechanism is presented in Fig. 2. For comparison, this figure also contains the DAE solution with no energy correction and the solution obtained using Baumgarte's constraint stabilization. In addition, we have derived an unconstrained equation of motion for the slider-crank mechanism,

$$\ddot{\theta}_1 + \frac{3}{5 - 3\cos(2\theta_1)} \left(\sin(2\theta_1)\dot{\theta}_1^2 + \frac{g}{l}\cos(\theta_1) \right) = 0 \quad (24)$$

(where θ_1 is the absolute angle of the base link measured counterclockwise from a horizontal reference). This equation was used to

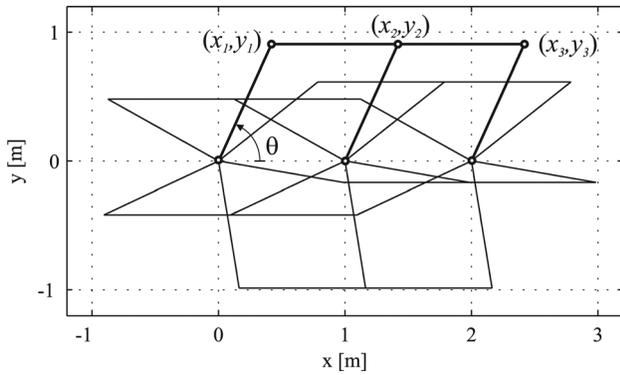


Fig. 5 Double four-bar linkage: $l = 1m$, $m = 1$ kg for each link. Whenever the links become horizontal, $y_1 = y_2 = y_3 = 0$, the linkage moves through a kinematic singularity.

define the numerically exact ODE solution, and an additional ODE solution obtained using the same fixed step RK4 solver employed for the proposed DAE integration. Note that with the large time step used, only the combined constraint and energy correction provide accurate solution.

Figure 3 depicts the constraint error, energy error and the overall error calculated along the previously defined numerical solutions. By applying the presented constraint correction, the motion constraints are precisely and steadily maintained, while the additional energy correction prevents energy drift. Figure 3(d) further shows that while in short and moderately long integrations, the energy correction may not be essential for precision, in long simulations the energy conserving DAE integrator can significantly enhance accuracy. More specifically, the proposed explicit DAE method can maintain higher precision than one could obtain using even an unconstrained formulation integrated with the same ODE solver.

In Fig. 4, we characterize the relation between accuracy and step size for solutions obtained with the proposed explicit DAE integrator. If a small enough step size is used, the overall error obtained with the proposed integrator is the same (or lower) than the error obtained with the unconstrained formulation integrated with the same ODE solver. With larger time steps, however, the proposed DAE solution, enhanced with the described energy correction, maintains a considerably improved accuracy level, relative to a corresponding ODE formulation, see Fig. 4(d). Compared to the energetically uncorrected DAE solution, application

of the energy correction makes the integration only slightly more expensive, see Fig. 4(e).

4.2 Double Four-Bar Linkage. Consider the double four-bar linkage with links of length l and distributed masses m , see Fig. 5. This example is selected to demonstrate a precise long-time energy conserving DAE integration through kinematic singularities.

The linkage is modeled as a constrained system using six coordinates which define the position of the moving joints $\mathbf{q} = [x_1, y_1, x_2, y_2, x_3, y_3]^T$. The equation of the unconstrained motion, $\mathbf{M}\ddot{\mathbf{q}} = \mathbf{Q}$, is given by

$$\begin{bmatrix} \frac{2}{3}m & 0 & \frac{1}{6}m & 0 & 0 & 0 \\ 0 & \frac{2}{3}m & 0 & \frac{1}{6}m & 0 & 0 \\ \frac{1}{6}m & 0 & m & 0 & \frac{1}{6}m & 0 \\ 0 & \frac{1}{6}m & 0 & m & 0 & \frac{1}{6}m \\ 0 & 0 & \frac{1}{6}m & 0 & \frac{2}{3}m & 0 \\ 0 & 0 & 0 & \frac{1}{6}m & 0 & \frac{2}{3}m \end{bmatrix} \begin{bmatrix} \ddot{x}_1 \\ \ddot{y}_1 \\ \ddot{x}_2 \\ \ddot{y}_2 \\ \ddot{x}_3 \\ \ddot{y}_3 \end{bmatrix} = \begin{bmatrix} 0 \\ -mg \\ 0 \\ \frac{3}{2}mg \\ 0 \\ -mg \end{bmatrix}$$

the holonomic kinematic constraints are

$$\Phi_q = \begin{bmatrix} x_1^2 + y_1^2 - l^2 \\ (x_2 - l)^2 + y_2^2 - l^2 \\ (x_3 - 2l)^2 + y_3^2 - l^2 \\ (x_2 - x_1)^2 + (y_2 - y_1)^2 - l^2 \\ (x_3 - x_2)^2 + (y_3 - y_2)^2 - l^2 \end{bmatrix} = \mathbf{0}$$

while the energy conservation law is given as

$$\Phi_e = \frac{1}{2} \dot{\mathbf{q}}^T \mathbf{M} \dot{\mathbf{q}} + mg \left(y_1 + \frac{3}{2} y_2 + y_3 \right) - E_0 = 0$$

Figure 6 shows the solution obtained with the proposed explicit DAE integrator and with Baumgarte's constraint stabilization. Alternative ODE solutions are also presented for accuracy assessment. Note that during such long time simulation (i.e., 1000 s), performed with a relatively large time step (i.e., 10^{-2} s), only the

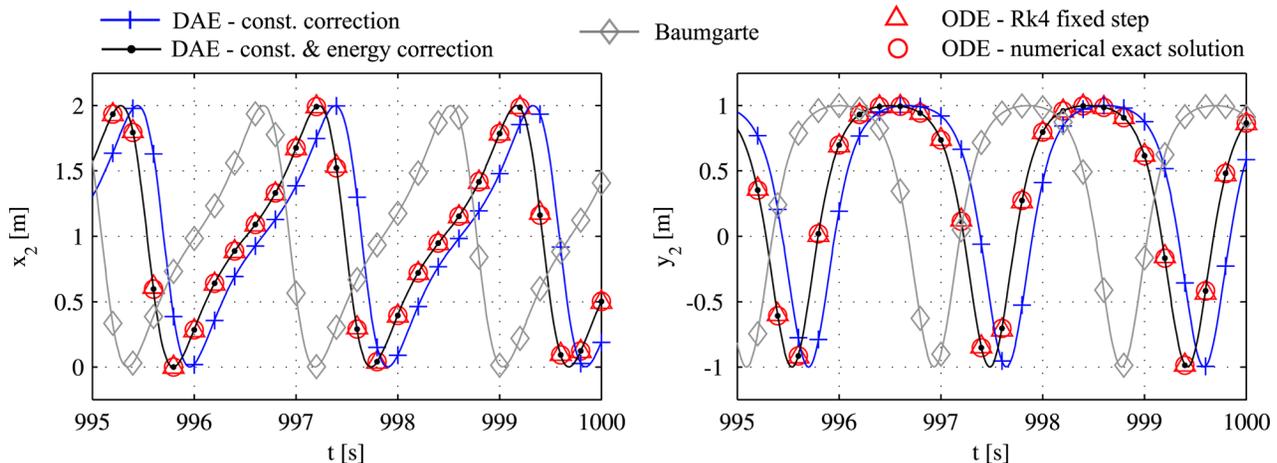


Fig. 6 Double four-bar linkage: $l = 1m$, $m = 1$ kg for each link. The simulations are performed through $t \in [0, 1000]$ s, with time step 10^{-2} s and $\mathbf{q}(0) = [0, 1, 1, 1, 2, 1]^T$, $\mathbf{v}(0) = [1, 0, 1, 0, 1, 0]^T$. The ODE solutions are obtained using the unconstrained formulation of the problem: $\ddot{\theta} + (7g/6l)\cos(\theta) = 0$, $\theta(0) = \pi/2$, $\dot{\theta}(0) = -1$ (θ denotes the orientation of the base link, see Fig. 5).

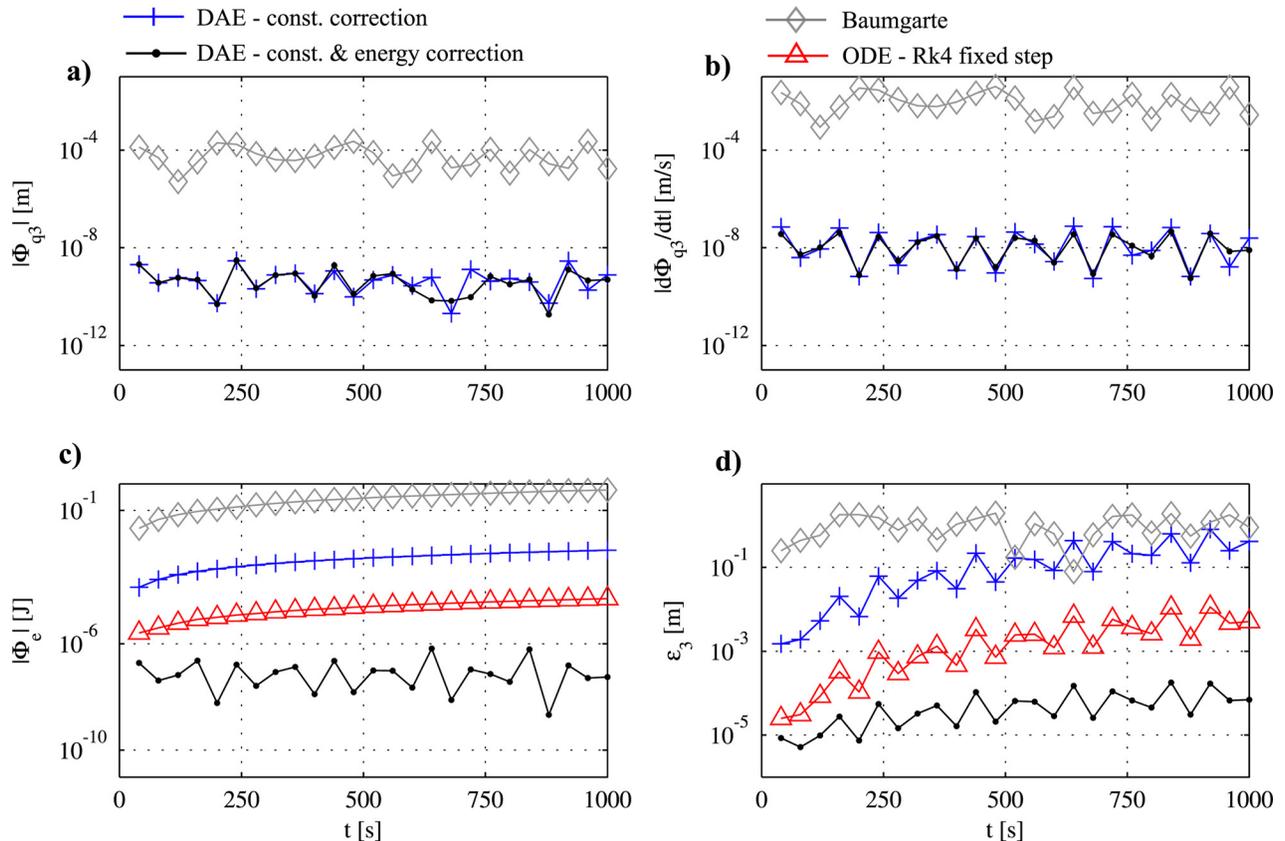


Fig. 7 Evolution of the (least accurate) kinematic constraints, the energy conservation law and the overall accuracy $\epsilon_3 = \sqrt{dx_3^2 + dy_3^2}$ where dx_3, dy_3 is measured between the solutions depicted in Fig. 6, and the numerically exact solutions for (x_3, y_3)

energetically corrected DAE integration provides an accurate solution.

Figure 7 depicts the kinematic constraint error, the error with respect to the energy conservation law, and the overall error calculated between the numerically exact solution and the solutions depicted in Fig. 6. One can see that the kinematic constraints are steadily maintained, and the energy drift is also prevented. Further, the overlap between the DAE solutions obtained with and without energy correction in Figs. 7(a) and 7(b) [and also in Figs. 3(a) and 3(b)] demonstrates that the proposed energy correction does not interfere with the kinematic constraint correction. Finally, Fig. 7(d) shows that the proposed DAE solution remains accurate despite the long time integration and despite movement through kinematic singularities.

5 Conclusion

This paper presents an equation of motion derived to enable the effective explicit numerical integration of constrained dynamical systems modeled with holonomic and nonholonomic kinematic constraints. The derivation is performed by assuming that the numerical solution is error contaminated, such that neither the kinematic constraints nor the energy conservation law can be exactly satisfied. Due to these practical limitations, the proposed equation of motion contains embedded terms that perform continuous constraint correction and also energy correction during the simulation. The equation can be directly discretized and solved with standard explicit ODE solvers, and it also provides a viable simulation tool even if the constraint set is redundant or if the system moves through kinematic singularities. Beyond the presented examples, implementation and application of the present formulation is further demonstrated in Part II of this work.

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