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Explicit symplectic momentum-conserving time-stepping scheme for the dynamics of geometrically exact rods

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ABSTRACT

A new structure-preserving algorithm for simulating the nonlinear dynamics of geometrically exact rods is developed. The method is based on the simultaneous discretization in space and time of Hamilton's variational principle. The resulting variational integrator is explicit, second-order accurate and can be identified with a Lie-group symplectic partitioned Runge–Kutta method for finite element discretizations of rods involving large rotations and displacements. Numerical examples allow to verify that the algorithm presents an excellent long term energy behavior along with the exact conservation of the momenta associated to the symmetries of the system.

1. Introduction

The formulation of continuum based theories for rods has captured the interest of researchers during decades [60]. The motivation for developing such theories is rooted in attempting to model complex physical problems arising in the dynamics of slender solids by means of a dimensionally reduced approach. This point of view has boosted the construction of models depending on one spatial variable and the time [1,73].

One of the most successful models[1] for describing the dynamics of elastic rods undergoing finite deformation has been proposed by Simo in [65]. This geometrically exact formulation follows a director-type approach to describe the kinematics of the rods and corresponds to a three-dimensional generalization of Reissner's original model [60,61]. In a posterior work, Simo and Vu-Quoc [69,70] proposed a numerical scheme based on combining the finite element method (FEM) with a modified version of Newmark's scheme for time integration. Other authors have also made highlighting contributions. For example, an initially curved reference configuration for the rod has been considered in [31,32,37]. A total Lagrangian formulation has been proposed in [11] and revisited in [47]. Some important numerical issues such as the construction of non-locking elements or frame-indifferent formulations can be consulted in [8,35,62,63]. An alternative formulation based on some concepts of geometric (Clifford) algebra is presented in [58]. The list of works largely exceeds the mentioned ones, which only constitute some relevant examples; a more complete survey can be consulted in [53].

From the point of view of the applications, this formulation has also received considerable attention. In [72] Simo and Vu-Quoc applied the model to study the dynamics of earth-orbiting flexible satellites with multibody components. It has also been used for studying the dynamics of flexible mechanisms [7,10], robotic technology [78], the coupled geometric and constitutive nonlinear response of structures and buildings in the static [56] and dynamic cases [57], including applications to passive control in earthquake engineering [73,53]. The application of the model to the study of slender structures made of composite materials has been carried out in [75–77].

The formulation of time integrators for the Reissner–Simo theory of elastic rods results to be a particularly challenging task since the model describes a dynamical system evolving on a nonlinear manifold rather than on a linear space. Several approaches have been proposed in order to design time integrators respecting the geometry of the configuration space. The design of structure-preserving algorithms for dynamics of rigid bodies is closely linked to the design of new methods for elastic rods. In this sense, Simo and Wong [71] developed a midpoint algorithm on $SO(3)$[2] which conserves the total

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[1] An alternative to geometrically exact models is given by the *co-rotational approach* for rods, see for example [15].

[2] The symbol $SO(3)$ denotes the non-commutative group of proper rotations [47].

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energy and the norm of the total momentum. They also formulated an implicit energy and momentum conserving algorithm. In [70] Newmark's method was extended to include $SO(3)$ yielding to a scheme able to handle arbitrarily large rotations and displacements. Even though this scheme has demonstrated to be useful in several applications [11], Mäkinen states [46] that it only constitutes an approximated version of the correct formulas, which are given in [2].

In spite of the above results, it is widely recognized that Newmark's family of implicit schemes fails to preserve the invariants of nonlinear Hamiltonian systems with symmetry [68]. Moreover, the stability and accuracy properties are not guaranteed in the nonlinear range [3,4]. A further step towards the development of robust schemes is given by formulation of the so-called the energy and momentum conserving (E–M) methods. They have been extended to elastic rods by Simo et al. in [67]. An alternative to E–M methods is given by the *symplectic-momentum* methods which are characterized by the preservation of certain skew-symmetric bilinear form on the phase space[3] along with the exact conservation of the momenta associated to symmetries of the Lagrangian. A comparison between symplectic and E–M schemes is presented in [24]. First-order accurate algorithms that exhibit controllable energy dissipation and momentum conservation are formulated in [3] and second-order methods can be found in [4].

More recently, the attention have been turned towards the so-called *variational integrators* (VI) which are methods obtained from a discrete version of Hamilton's principle for conservative systems [51,52,59,79]. These methods present remarkable properties among which are: (i) they are symplectic, (ii) they exactly conserve the momenta associated to the symmetries of a discrete Lagrangian and (iii) they show an excellent long time energy behavior. Moreover, higher order methods can be constructed following a systematic procedure. An overview of the method can be found in [44] and the case of continuum systems in considered in [49,81]. The construction of asynchronous VI's is carried out in [43] and development of generalized Galerkin VI's, including dynamical systems evolving on Lie groups, can be consulted in [41,39,40]. In summary, variational methods constitute an extraordinarily versatile framework for the systematic construction of structure-preserving time integrators [29] that can be applied to a wide variety of problems arising in different fields of science and engineering [41,55]. However, the variational techniques have not been applied to formulate structure-preserving methods for geometrically exact rods.

Innovative numerical models of elastic rods are currently used in a wide range of subjects areas such as computational biophysics, the dynamics of interacting biomolecules and filaments, synthetic polymers and new materials based on nano-technologies. For example, in [38] a numerical model for the dynamics of viscous Kirchhoff rods is used for studying problems of biological significance, including the super-coiling and instability in closed rods and the self-assembly behavior of fibril structures such as certain types of bacteria. Goriely and Tabor [25–27] study certain theoretical aspects of Kirchhoff's rods with applications in the numerical simulation of thin filaments. The application of rod models to the study the growth of certain plants can be consulted in [28]. In [23] a theory of elastic filaments is extended to consider biological systems that display competition between two helical structures of opposite chirality. Balaeff et al. [6] extend the classical Kirchhoff's model applied to deoxyribonucleic acid (DNA) to account for sequence-dependent intrinsic twist and curvature, anisotropic rotational stiffness and electrostatic interactions. Yang et al. [80] construct a finite element (FE) model for inextensible elastic rods including self-contact and use it for modelling a DNA polymer composed of thousands of base pairs. A survey about the numerical modelling of super-helical DNA can be consulted in [64]. Therefore, it is necessary to formulate robust time integrators for simulating the dynamics of rods undergoing complex morphological changes.

In this work, a new explicit variational integrator for simulating the dynamics of geometrically exact rods is formulated. Its construction is built on the simultaneous discretization in space and time of the action functional. To this end, the finite element method is applied the continuum problem to obtain a finite-dimensional semi-discrete problem. Then, standard procedures in variational integration are applied on the nodal variables of the mesh to formulate a structure-preserving Lie-group partitioned Runge–Kutta method. The new time integrator enjoys a number of remarkable features: (i) it is explicit if an appropriate quadrature rule is used to compute the discrete kinetic energy, (ii) it is symplectic, (iii) it exactly conserves the momenta associated to the symmetries of the discrete Lagrangian, (iv) it is second-order accurate, (v) it shows an energy drift that remains bounded over exponentially long periods of times and, (vi) since it is explicit, it avoids using iterative schemes to solve large systems of nonlinear equations.

2. Geometrically exact rods

In this section the Lagrangian point of view of the mechanics is considered to deduce the balance equations for geometrically exact rods in finite deformation. Special emphasis is given to the non-linear nature of the configuration manifold. Additionally, the Hamiltonian structure of the problem is also addressed along with the invariants of the dynamics.

2.1. Model description

Kinematics: Let $\{\mathbf{E}_i\}$ and $\{\mathbf{e}_i\}$ be the *material* and *spatial* inertial frames, which are orthogonal and coincident.[4] The reference configuration is given by a straight rod of length L with constant cross section $\mathcal{A} \subset \mathbb{R}^2$. Then, the position vector of a material point in this configuration is

$$\mathbf{X}(s, \xi_1, \xi_2) = s\mathbf{E}_1 + \xi_1\mathbf{E}_1 + \xi_2\mathbf{E}_2,$$

where $s \in [0, L]$ is an arch-length coordinate and $(\xi_1, \xi_2) \in \mathcal{A}$ are coordinates on the cross section. The reference curve $\boldsymbol{\varphi}_0$ is defined as the geometric place of all the points of the form $\mathbf{X}(s, 0, 0)$. The position vector of a material point in the current configuration is given by

$$\mathbf{x}(s, \xi_1, \xi_2) = \boldsymbol{\varphi}(s) + \xi_1\mathbf{t}_1(s) + \xi_2\mathbf{t}_2(s), \tag{1}$$

where the spatial curve $\boldsymbol{\varphi} : [0, L] \to \mathbb{R}^3$ is obtained by adding a displacement onto $\boldsymbol{\varphi}_0$ and the vectors $\mathbf{t}_i = \boldsymbol{\Lambda}\mathbf{E}_i$ with $\boldsymbol{\Lambda} : [0, L] \to SO(3)$ define an orthonormal coordinate system characterizing the current orientation of the cross-section [65,37], see Fig. 1.

The *configuration space*, $\mathcal{Q}$, is the set of all the smooth-enough fields

$$\boldsymbol{\Phi} \equiv (\boldsymbol{\varphi}, \boldsymbol{\Lambda}) : [0, L] \to \mathbb{R}^3 \times SO(3), \tag{2}$$

subjected to the prescribed boundary conditions $\boldsymbol{\Phi}(0) = \boldsymbol{\Phi}_0$ and $\boldsymbol{\Phi}(L) = \boldsymbol{\Phi}_L$ and to the restriction $\boldsymbol{\varphi}_{,s} \cdot \mathbf{t}_1 > 0$ [67]. Due to the non-commutative nature of $SO(3)$, $\mathcal{Q}$ results to be a nonlinear differentiable manifold [50,68]. Thereby, using the spatial rule to update

[3] The simultaneous conservation of the total energy and the symplectic structure is not possible for methods with constant time step [36,41,22].

[4] Notation: Latin and Greek indexes range over {1,2,3} and {2,3}, respectively. The symbols $(\bullet)_{,x}$, $(\dot{\bullet})$ and $SO(3)$ denote differentiation with respect to x, time differentiation and the linear space of skew-symmetric tensors, respectively.