Energy-consistent integration of mechanical systems based on Livens principle

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EXTENDED ABSTRACT

1 Overview

In this work we make us of Livens principle (sometimes also referred to as Hamilton-Pontryagin principle) in order to obtain a novel structure-preserving integration scheme for mechanical systems. In contrast to the canonical Hamiltonian equations of motion, the Euler-Lagrange equations pertaining to Livens principle circumvent the need to invert the mass matrix. This is an essential advantage with respect to singular mass matrices, which can yield severe difficulties for the modelling and simulation of multibody systems (see, for example, Udwadia & Phohomsiri [1] and García de Jalón & Gutiérrez [2]). Moreover, Livens principle unifies both Lagrangian and Hamiltonian viewpoints on mechanics. Additionally, the present framework avoids the need to know the system's Hamiltonian. The novel scheme algorithmically conserves a general energy function and aims at the preservation of momentum maps corresponding to symmetries of the system. The performance of the newly devised method is studied in representative examples.

2 Hamiltonian dynamics

Consider the motion of a dynamical system with d degrees of freedom with positions $q \in Q$ and velocities $\dot{q} \in T_q Q$, where $Q \subset \mathbb{R}^d$ denotes the configuration space and $T_q Q \subset \mathbb{R}^d$ the tangent space to Q at q. The system's Lagrangian $L : TQ \to \mathbb{R}$ is given by

$$L(q,\dot{q}) = T(q,\dot{q}) - V(q) = \frac{1}{2}\dot{q} \cdot M(q)\dot{q} - V(q) \,, \tag{1}$$

where $T : TQ \to \mathbb{R}$ is the kinetic energy, $M(q) \in \mathbb{R}^{d \times d}$ denotes the symmetric and positive-semidefinite mass matrix and $V : Q \to \mathbb{R}$ is a potential function. The corresponding Hamiltonian $H : T^*Q \to \mathbb{R}$ can be obtained by employing a Legendre transformation $\mathbb{F}_L : (q,\dot{q}) \mapsto (q,p)$, where $p := D_2 L(q,\dot{q})$ are the conjugate momenta, such that

$$H(q,p) = p \cdot \dot{q}(q,p) - L(q,\dot{q}(q,p)) \,. \tag{2}$$

Given a Lagrangian (1), the Hamiltonian reads $H(q,p) = T(q,p) + V(q) = \frac{1}{2}p \cdot M(q)^{-1}p + V(q)$. Correspondingly, the Hamiltonian equations of motion appear in their canonical form

$$\dot{q} = D_2 H(q,p) \quad = M(q)^{-1}p \,, \tag{3a}$$

$$\dot{p} = -D_1 H(q,p) = -D_1 T(q,p) - DV(q) \,. \tag{3b}$$

However, this approach is limited to systems, for which a Hamiltonian can be found and the mass matrix is non-singular. Thus, we now want to introduce a different and more general framework.

3 Livens principle

From Hamilton's principle of least action one can proceed by allowing the velocities to be independent variables $v \in \mathbb{R}^d$. The kinematic relation $\dot{q} = v$ can be enforced by means of Lagrange multipliers $p \in \mathbb{R}^d$. The corresponding augmented action integral for the simulation time $t \in [0,T]$ reads

$$S(q,v,p) = \int_0^T \left[L(q,v) + p \cdot (\dot{q} - v) \right] \mathrm{d}t \tag{4}$$

and is called *Livens principle*. By stating the stationary condition $\delta S(q,v,p) = 0$ and executing the variations with respect to every independent variable, one obtains the equations of motion

$$\dot{q} = v \,, \tag{5a}$$

$$\dot{p} = D_1 L(q,v) \,, \tag{5b}$$

$$p = D_2 L(q,v) \,. \tag{5c}$$

With regard to (5c) the Lagrange multiplier p can be identified as the conjugate momentum. Thus, Livens principle automatically accounts for the Legendre transformation (2), whereas within the framework of Hamiltonian dynamics momentum variables have to be defined a priori using the fiber derivative. In analogy to (2), a generalized energy function

$$E(q,v,p) = p \cdot v - L(q,v) \tag{6}$$

can be introduced. It can be shown that the generalized energy is conserved along solutions of (5), i.e. $\mathrm{d}E/\mathrm{d}t = 0$.

Note that after reinserting (5c) into (5b) and making use of (5a), Livens principle traces back to the Lagrangian equations of the second kind. For mechanical systems with Lagrangian (1), relation (5c) yields $p = M(q)v$, so that, if M is nonsingular, (5a) and (5b) directly lead to the canonical Hamiltonian equations of motion (3). Moreover, the generalized energy function can be identified as the Hamiltonian, such that $E(q,v(q,p),p) = H(q,p)$.

Initially termed Livens principle (cf. Sec. 26.2 in Pars [3]) after G.H. Livens, who proposed this functional for the first time (cf. Livens [4]), later also the name *Hamilton-Pontryagin principle* has been coined for functional (4). More recently, preliminary works [5, 6] by the authors of this constribution have taken up Livens principle in order to obtain a novel variational principle, the *GGL principle* which extends Livens principle to holonomically constrained systems. In these works, new structure-preserving integrators for systems with constant mass matrix have been developed.

4 Structure-preserving discretization

In this work, a novel integration method is proposed, which conserves first integrals of the equations of motion at hand, e.g. the generalized energy function E. This scheme results from a direct discretization of the Euler-Lagrange equations (5) emanating from Livens principle. Particularly, discrete derivatives $\overline{\mathrm{D}} : \mathbb{R}^m \times \mathbb{R}^m \to \mathbb{R}^m$ in the sense of Gonzalez [7] are taken into account. Those discrete derivatives represent second-order approximation to the exact gradients such that for a given function $f : \mathbb{R}^m \to \mathbb{R}$ we have

$$\overline{\mathrm{D}}f(x,y) = \mathrm{D}f(z) + \frac{f(y) - f(x) - \mathrm{D}f(z) \cdot v}{||v||^2} v \tag{7}$$

with $z = (x+y)/2$, $v = y - x$ and $|| \bullet ||$ denoting the standard Euclidean norm on $\mathbb{R}^m$. Discrete derivatives satisfy the directionality condition $\overline{\mathrm{D}}f(x,y) \cdot v = f(y) - f(x)$ as well as the consistency condition $\overline{\mathrm{D}}f(x,y) = \mathrm{D}f(z) + O(||v||)$. Correspondingly, partitioned discrete derivatives can be defined.

5 Conclusion

The newly proposed structure-preserving integration schesme differs from the method presented by Gonzalez [7] with respect to the formulation in a more general (not necessarily Hamiltonian) framework. Thus, the need for the inversion of the mass matrix is avoided, which circumvents numerical instabilities near singular configurations. The method discretely covers the conservation of the generalized energy (6), i.e. $E^{n+1} = E^n$ and aims at the preservation of momentum maps corresponding to the system's symmetries. It can be observed, that the integrator is second-order accurate. The presented framework can be extended to mechanical systems subject to holonomic constraints.

Acknowledgments

References

[1] F. Udwadia and P. Phohomsiri. Explicit equations of motion for constrained mechanical systems with singular mass matrices and applications to multi-body dynamics. Proceedings of the Royal Society A, 462: 2097–2117, 2006.

[2] J. García de Jalón and M. D. Gutiérrez-López. Multibody dynamics with redundant constraints and singular mass matrix: existence, uniqueness, and determination of solutions for accelerations and constraint forces. Multibody System Dynamics, 30(3): 311–341, 2013.

[3] L. A. Pars. A treatise on analytical dynamics. The Mathematical Gazette, 50(372): 226–227, 1966.

[4] G. H. Livens. IX. – On Hamilton's principle and the modified function in analytical dynamics. Proceedings of the Royal Society Edinburgh, 39: 113–119, 1919.

[5] P. L. Kinon, P. Betsch and S. Schneider. The GGL Variational Principle for Constrained Mechanical Systems. Accepted for publication in Multibody System Dynamics, 2022.

[6] P. L. Kinon, P. Betsch and S. Schneider. Structure-preserving integrators based on a new variational principle for constrained mechanical systems. Nonlinear Dynamics (under revision), 2022.

[7] O. Gonzalez. Time integration and discrete Hamiltonian systems. Journal of Nonlinear Science, 6: 449–467, 1996.