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# Exploring the Benefits of Variational Integrators with Natural Coordinates: A Pendulum Example.

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**EXTENDED ABSTRACT**

## 1 Introduction

Using natural coordinates in biomechanics is particularly beneficial [1, 2] because they can directly derive from landmarks' locations in the global frame, measured with motion capture systems. For inverse kinematics, natural coordinates lead to a set of linear or quadratic constraints that are easy to solve. They can also describe complex joints to better fit the anatomical structures [3]. For example, the knee joint can be modeled with ligament constraints and sphere-on-plane joints for the contact between femur condyles and the tibial plateau instead of a simplistic hinge. This formalism is convenient for inverse dynamics but rarely used in forward dynamics, especially in an optimal control scheme, for which minimal coordinates are preferred.

The challenge comes from constrained dynamics which results in index-1 differential algebraic equations (DAE), see Eq. (3), and Eq. (4). Their integration produces a numerical drift that violates the original constraints. Using Baumgarte's stabilization is one solution, but it usually adds extra energy to the system that ultimately breaks the physics [4]. Variational integrators might be an option because they obey constraints and are symplectic by construction [5]. Unlike traditional differential equation solvers (e.g., Runge-Kutta (RK) schemes), they conserve energy and rely on discrete dynamics.

We propose to review the concept of variational integrators using a natural coordinates formalism for mechanical and biomechanical applications. Then our main objective is to assess the effectiveness of our proposed variational integrators compared to traditional ODE solvers.

## 2 Background

**Formalism.** As proposed for numerous biomechanics analyses [1, 2], the $n$-th segment in a multibody system with $N$ segments has generalized coordinates with two points and directions: $\mathbf{q}_n = \left(\mathbf{u}_n, \mathbf{r}_{p_n}, \mathbf{r}_{d_n}, \mathbf{w}_n\right)^\top \in \mathbf{R}^3 \times \mathbf{R}^3 \times \mathbf{R}^3 \times \mathbf{R}^3$, where $\mathbf{u}$, $\mathbf{r}_p$, $\mathbf{r}_d$, and $\mathbf{w}$ are, respectively, the proximal vector, the position of the proximal point, the position of the distal point, and the distal vector, all expressed in the global coordinate system. The generalized coordinates of the whole system are $\mathbf{q} = (\mathbf{q}_1, \ldots, \mathbf{q}_N)^\top \in \mathbf{R}^{12\times N}$. Two types of holonomic constraints are handled in this formalism: rigid-body constraints and joint constraints (also termed as kinematic constraints), denoted $\Phi^r(\mathbf{q})$ and $\Phi^j(\mathbf{q})$, respectively, and gathered in a common constraint function $\Phi$:

$$\Phi(\mathbf{q}) = \begin{pmatrix}\Phi^r(\mathbf{q}) & \Phi^j(\mathbf{q})\end{pmatrix}^\top \in \mathbf{R}^{6\times N} \times \mathbf{R}^M. \tag{1}$$

**Continuous equations of motions.** Given the multibody system's Lagrangian function $L(\mathbf{q},\dot{\mathbf{q}}) = T(\dot{\mathbf{q}}) - V(\mathbf{q})$, the least action principle states that the state trajectory is a stationary point of the action function defined by:

$$S(\mathbf{q}) = \int_0^T L(\mathbf{q},\dot{\mathbf{q}})dt \tag{2}$$

In continuous time, the stationary conditions lead to the classical constrained Euler-Lagrange equations:

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{\mathbf{q}}} - \frac{\partial L}{\partial \mathbf{q}} = \mathbf{K}(\mathbf{q})^\top \lambda \tag{3a}$$

$$\Phi(\mathbf{q}) = 0 \tag{3b}$$

where $\mathbf{G}$, $\mathbf{K}(\mathbf{q})$ stand for the constant generalized mass matrix, and the Jacobian constraint of $\Phi(\mathbf{q})$. The Lagrange multipliers $\lambda \in \mathbf{R}^{6\times N+M}$ are the forces that hold the system together. By differentiating twice Eq. (3b), Eq. (3) can be reduced into its index-1 DAE form:

$$\begin{bmatrix}\mathbf{G} & \mathbf{K}(\mathbf{q})^\top \\ \mathbf{K}(\mathbf{q}) & 0\end{bmatrix}\begin{pmatrix}\ddot{\mathbf{q}} \\ \lambda\end{pmatrix} = \begin{pmatrix}0 \\ -\dot{\mathbf{K}}(\mathbf{q})\dot{\mathbf{q}}\end{pmatrix} \tag{4}$$

**Discrete equations of motions.** By discretizing Eq. (2), it introduces a discrete version of the variational principle [5]:

$$S^d(\mathbf{q}_d) = \sum_{i=0}^{N_f-1}\int_{t_i}^{t_{i+1}} L(\mathbf{q},\dot{\mathbf{q}})dt = \sum_{i=0}^{N_f-1}\frac{\Delta t}{2}L\left(\mathbf{q}^i, \frac{\mathbf{q}^{i+1}-\mathbf{q}^i}{\Delta t}\right) + \frac{\Delta t}{2}L\left(\mathbf{q}^{i+1}, \frac{\mathbf{q}^{i+1}-\mathbf{q}^i}{\Delta t}\right) = \sum_{i=0}^{N_f-1} L_d(\mathbf{q}^i,\mathbf{q}^{i+1}) \tag{5}$$

where $L_d(\mathbf{q}^i, \mathbf{q}^{i+1})$ is a term for the quadrature of the action integral approximated by a trapezoidal rule, and $\mathbf{q}_d$ is the generalized coordinates for all the discrete instant of time such that $\mathbf{q}_d = [\mathbf{q}^0, \cdots, \mathbf{q}^{N_f}]$. Looking at the stationary conditions, it leads to the so-called *Constrained Discrete Euler-Lagrange equations* (CDEL):

$$\partial_2 L_d(\mathbf{q}^{i-1}, \mathbf{q}^i) + \partial_1 L_d(\mathbf{q}^i, \mathbf{q}^{i+1}) - \mathbf{K}^\top(\mathbf{q}^i)\lambda^i = 0 \tag{6}$$

$$\Phi(\mathbf{q}^{i+1}) = 0 \tag{7}$$

Thus, we have $12 \times N + 6 \times N + M$ equations to solve with $\mathbf{q}^{i+1}$ and $\lambda^i$ as unknown variables. The root-finding Newton-Raphson algorithm can solve Eq. (6) and (7) for each iteration.

## 3 Material and Methods

A 20-segment planar pendulum was modeled with 20 hinges. Each segment was described with 12 coordinates as presented in the background. This multibody system is assumed to be representative of a biomechanical system. The index-1 DAE and the CDEL equations were considered to simulate the dropped pendulum during 15 s. The index-1 DAE was integrated using a fixed-step 4th-order Runge-Kutta (RK4) ordinary differential equation solver, a variable-step Runge-Kutta of order 5(4) (RK45), and the CDEL equations were solved with a Newton-Raphson algorithm. Time steps were set to 0.04 s. The initial conditions set the pendulum to the horizontal without initial velocity so that the initial total energy was 0 J. The initial second-time step was evaluated with the generalized coordinates from the RK45 computation, to start the variational integrator. The source code can be found at github.com/Ipuch/variational_integrator. It was implemented with the package github.com/Ipuch/bionc interfaced with CasAdi to compute all the derivatives. To compare the consistency of the simulations, rigid-body and joint constraints residuals, and the total energy of the system were reported.

## 4 Results

Table 1: Total Energy, rigid-body constraints, and joint constraints residuals after 15 seconds of integration.

| | Total Energy (J) | Rigid-body constraints $\Phi^r(\mathbf{q})$ median (min - max) | Joints constraints $\Phi^j(\mathbf{q})$ median (min - max) |
|---|---|---|---|
| Runge-Kutta 45 | 822 | $1.4e^{-16}$ ( $-7.5e^{-3}$ - $3.9e^{-2}$ ) | 0.0 ($-8.8e^{-13}$ - $1.1e^{-13}$) |
| Variational integrator | 0.01 | $6.5e^{-25}$ ($-1.6e^{-17}$ - $2.0e^{-12}$) | 0.0 ($-1.2e^{-22}$ - $5.7e^{-23}$) |

The RK4 solver diverged, and the generalized coordinates reached infinity. Other results after 15 s of integration are reported in Table 1. The RK45 modified the total energy by the end of the simulation from 0 to 822 J. Rigid-body constraints were less satisfied than joint constraints, magnitude orders ranged from $-1e^{-3}$ to $1e^{-2}$. The variational integrator preserved the system's energy at 0.01 J. Rigid-body constraints and joint constraints were satisfied within a maximum order of magnitude of $1e^{-12}$.

## 5 Discussion

We have shown that our variational integrator can be used with a natural coordinates formalism, and typically for biomechanics. The variational integrator performed better than the traditional RK4 and RK45 solvers in terms of accuracy and stability. Even if RK45 was correct in ensuring the holonomic constraints, it might not perform as well with joints more complex than hinges. As previously shown, variational integrators preserve the system's energy for mechanics formalisms such as minimal, maximal, or natural coordinates, including this study. The strengths of variational integrators need to be acknowledged: first, the preservation of the energy is independent of the time steps, as opposed to other RK integrators; second, as it is a fixed-step integrator, it is adapted for optimal control approaches. This could benefit for optimal estimation of muscle forces with musculoskeletal models. Further research is needed to extend this approach to more complex biomechanical models and to use it with experimental data.

## References


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