A Moreau-type Variational Integrator

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In this paper we derive a variational integrator for nonsmooth mechanical systems by discretizing the principle of virtual action with finite elements in time. After the discretization with local finite elements, the constitutive laws for the contact forces are introduced as in Moreau's time stepping scheme. This derivation shows exemplary how variational integrators for systems with frictional unilateral constraints can be derived. The long-time energy behavior of the presented scheme is compared with the behavior of Moreau's stepping scheme on an example system.

1 Introduction

Mechanical systems often exhibit a particular differential geometric structure and the study of these various properties for different classes of systems has a long tradition in mechanics. Hamiltonian systems, for example, are known to be symplectic and conserve the total mechanical energy. In addition to conservation properties, a mechanical system can also show time reversibility among other symmetries. These properties are of essential importance for the system behavior and it has proven to be useful to respect the underlying structure also in the numerical treatment of the system. Such so-called structure preserving numerical schemes are known to be very performing for long-time simulations and are very robust [1]. One possibility to construct structure preserving integrators is by discretizing a variational principle with finite elements in time, leading to a variational integrator [2]. By discretizing the principle of virtual action with finite elements in time and choosing the discrete constitutive contact law of Moreau, we derive in this paper a variational integrator for nonsmooth mechanical systems. Moreau's contact law describes frictional unilateral constraints between contacting bodies with Newton-type impact law and Coulomb friction law. It is suitable for problems with many contacts and can overcome accumulation points. Both the qualities of the variational integrators and the qualities of Moreau's contact law are therefore combined in the presented scheme. Subsequent to the derivation of the stepping scheme, the presented scheme is compared with Moreau's stepping scheme in terms of long-time energy behavior.

2 Time-Continuous System

Consider the motion of a mechanical system $\mathcal{S}$ during the time interval $\mathcal{I} = [0, T]$, which is parametrized by the time t and a set of generalized coordinates $\boldsymbol{q}(t) \in \mathbb{R}^n$. Let $\dot{\boldsymbol{q}}(t) \in \mathbb{R}^n$ denote the corresponding generalized velocities of $\mathcal{S}$, where $\dot{(\bullet)} = \frac{\mathrm{d}}{\mathrm{d}t}(\bullet)$ denotes the derivation with respect to time. The variational family $\hat{\boldsymbol{q}}(t, \varepsilon)$, which contains the actual motion in the sense that $\hat{\boldsymbol{q}}(t, \varepsilon_0) = \boldsymbol{q}(t)$, is used to define the virtual displacements $\delta\boldsymbol{q}(t) = \frac{\partial \hat{\boldsymbol{q}}}{\partial \varepsilon}(t, \varepsilon_0)\delta\varepsilon$ with an infinitesimal variational parameter $\delta\varepsilon$. The system $\mathcal{S}$ is restricted by scleronomic geometric unilateral constraints, which are represented by the inequalities $g_j(\boldsymbol{q}) \geq 0$ $(j = 1, \ldots, n_c)$ with the gap functions g_j being zero in case of contact, positive in case of separation and negative when penetration occurs. On velocity level, the state of the contact is fully described by the normal and tangential contact velocities $\gamma_{N,j} = \dot{g}_j$ and $\boldsymbol{\gamma}_{T,j}$, respectively. The contact velocities induce the generalized directions $\boldsymbol{w}_{N,j} = (\frac{\partial \gamma_{N,j}}{\partial \dot{\boldsymbol{q}}})^{\mathrm{T}} = (\frac{\partial g_{N,j}}{\partial \boldsymbol{q}})^{\mathrm{T}}$ and $\boldsymbol{w}_{T,j} = (\frac{\partial \boldsymbol{\gamma}_{T,j}}{\partial \dot{\boldsymbol{q}}})^{\mathrm{T}}$, which are stored in the columns of the matrices $\boldsymbol{W}_B = (\boldsymbol{w}_{B,1}, \ldots, \boldsymbol{w}_{B,n_c})$ for $B \in \{N, T\}$ and $\boldsymbol{W} = (\boldsymbol{W}_N, \boldsymbol{W}_T)$. The virtual action of the system

$$\delta A(\delta\boldsymbol{q}) = \int_{\mathcal{I}} \left\{ \delta T(\boldsymbol{q}, \dot{\boldsymbol{q}}, t) + \delta\boldsymbol{q}^{\mathrm{T}} \left(\boldsymbol{f} + \boldsymbol{W}\boldsymbol{\lambda} \right) \right\} \mathrm{d}t + \sum_{i=1}^{m} \delta\boldsymbol{q}(t_i)^{\mathrm{T}} \boldsymbol{W}_i \boldsymbol{\Lambda}_i + \delta\boldsymbol{q}(0)^{\mathrm{T}} \boldsymbol{P}_0 - \delta\boldsymbol{q}(T)^{\mathrm{T}} \boldsymbol{P}_T \tag{1}$$

with $\boldsymbol{W}_i = \boldsymbol{W}|_{t_i}$ describes the dynamics of the system $\mathcal{S}$, where the inertia of the system is given by the variation of the kinetic energy $T(\boldsymbol{q}, \dot{\boldsymbol{q}}, t)$. Furthermore, the virtual action includes the effects of the contact forces $\boldsymbol{\lambda}$, various external forces $\boldsymbol{f}$ and impulsive contact forces $\boldsymbol{\Lambda}_i$, which act at a priori unknown but countably many time instants t_i. At the boundaries of the time interval $\mathcal{I}$ two impulsive forces, $\boldsymbol{P}_0$ and $\boldsymbol{P}_T$, are introduced, which are required to impose the initial conditions. Computing the variation of the kinetic energy in (1), i.e. $\delta T = \frac{\partial T}{\partial \boldsymbol{q}}\delta\boldsymbol{q} + \frac{\partial T}{\partial \dot{\boldsymbol{q}}}\delta\dot{\boldsymbol{q}}$, and applying integration by parts on every

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non-impulsive time interval (t_i, t_{i+1}) of the term containing $\delta\dot{\boldsymbol{q}}$, we obtain the strong variational form of the virtual action

$$\begin{aligned}\delta A(\delta\boldsymbol{q}) = &\sum_{i=0}^{m}\int_{t_i}^{t_{i+1}} \delta\boldsymbol{q}^{\mathrm{T}}\left[-\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial T}{\partial\dot{\boldsymbol{q}}}\right)^{\mathrm{T}} + \left(\frac{\partial T}{\partial\boldsymbol{q}}\right)^{\mathrm{T}} + \boldsymbol{f} + \boldsymbol{W}\boldsymbol{\lambda}\right]\mathrm{d}t - \delta\boldsymbol{q}(0)^{\mathrm{T}}\left[\left(\frac{\partial T}{\partial\dot{\boldsymbol{q}}}\right)^{\mathrm{T}}\Big|_{0^+} - \boldsymbol{P}_0\right] \\ &- \sum_{i=1}^{m}\delta\boldsymbol{q}(t_i)^{\mathrm{T}}\left[\left(\frac{\partial T}{\partial\dot{\boldsymbol{q}}}\right)^{\mathrm{T}}\Big|_{t_i^+} - \left(\frac{\partial T}{\partial\dot{\boldsymbol{q}}}\right)^{\mathrm{T}}\Big|_{t_i^-} - \boldsymbol{W}_i\boldsymbol{\Lambda}_i\right] + \delta\boldsymbol{q}(T)^{\mathrm{T}}\left[\left(\frac{\partial T}{\partial\dot{\boldsymbol{q}}}\right)^{\mathrm{T}}\Big|_{T^-} - \boldsymbol{P}_T\right],\end{aligned} \tag{2}$$

where the subscripts t^- and t^+ denote the left and right limits at t, respectively. The principle of virtual action postulates the virtual action to vanish for all virtual displacement fields $\delta\boldsymbol{q}(t)$. Applying this principle to the strong variational form of the virtual action (2) together with the fundamental lemma of calculus of variations, all terms in the square brackets have to vanish pointwise. This leads directly to the equations of motion for the non-impulsive time intervals, the impact equations for the time instants t_i and the boundary conditions. Choosing appropriate constitutive laws for the contact forces $\boldsymbol{\lambda}$ and contact impulses $\boldsymbol{\Lambda}_i$, the resulting nonsmooth system can be used to describe unilaterally constrained systems with frictional contacts, cf. [3]. A numerical approximation of the solution of such nonsmooth systems is derived in the next section.

3 Stepping Scheme

The dynamics of $\mathcal{S}$ is approximated numerically by a Bubnov–Galerkin approach in time. Introducing a uniform grid of N temporal nodes $(t_1, \ldots, t_N)$, the time interval $\mathcal{I}$ is subdivided into temporal elements $\Omega_k = [t_k, t_{k+1})$ of constant length $\Delta t = t_{k+1} - t_k$. For every element we approximate the motion by a local shape function given by the linear Lagrangian polynomial

$$\boldsymbol{q}(t) = (1 - s_k(t))\boldsymbol{q}_k + s_k(t)\boldsymbol{q}_{k+1} \quad \text{with} \quad s_k(t) = \frac{t - t_k}{\Delta t} \quad \text{for} \quad t \in \Omega_k\,. \tag{3}$$

The variation $\delta\boldsymbol{q}_k$ of the discrete coordinates $\boldsymbol{q}_k$ induce a virtual displacement field $\delta\boldsymbol{q}(t)$ admissible with respect to (3). For a discretization in the sense of Bubnov–Galerkin, we substitute $\boldsymbol{q}(t)$ in (1) by (3) and choose admissible virtual displacements. The global motion $\boldsymbol{q}(t)$ defined by (3) is absolutely continuous and piecewise linear in t. Therefore, the velocity $\dot{\boldsymbol{q}}(t)$ is piecewise constant with velocity jumps only at the temporal nodes t_k. It follows from the impact equations that the impulsive contact forces can only be non-zero for those time instants for which velocity jumps occur. Hence, the impulsive forces appear only at the temporal nodes. The integral over the time interval $\mathcal{I}$ is approximated numerically by applying the trapezoidal rule

$$\int_{t_k}^{t_{k+1}} h(t)\mathrm{d}t = \frac{\Delta t}{2}\big(h(t_k) + h(t_{k+1})\big) \tag{4}$$

in each temporal element Ω_k. For the computation of the discrete virtual action, the abbreviation $\boldsymbol{u}_k = (\boldsymbol{q}_{k+1} - \boldsymbol{q}_k)/\Delta t$ and the notations $T_{,\boldsymbol{q}} = (\frac{\partial T}{\partial\boldsymbol{q}})^{\mathrm{T}}$ and $T_{,\dot{\boldsymbol{q}}} = (\frac{\partial T}{\partial\dot{\boldsymbol{q}}})^{\mathrm{T}}$ are introduced. The discretization of the second term of the variation of the kinetic energy in (1) is

$$\begin{aligned}\sum_{k=1}^{N-1}\int_{t_k}^{t_{k+1}} \delta\dot{\boldsymbol{q}}^{\mathrm{T}}\boldsymbol{T}_{,\dot{\boldsymbol{q}}}(\boldsymbol{q},\dot{\boldsymbol{q}},t)\mathrm{d}t &\overset{(3)}{=} \sum_{k=1}^{N-1}\int_{t_k}^{t_{k+1}} \frac{1}{\Delta t}\big(\delta\boldsymbol{q}_{k+1} - \delta\boldsymbol{q}_k\big)^{\mathrm{T}}\boldsymbol{T}_{,\dot{\boldsymbol{q}}}\big((1-s_k)\boldsymbol{q}_k + s_k\boldsymbol{q}_{k+1}, \boldsymbol{u}_k, t\big)\mathrm{d}t \\ &\overset{(4)}{=} \sum_{k=1}^{N-1}\frac{1}{2}\big(\delta\boldsymbol{q}_{k+1} - \delta\boldsymbol{q}_k\big)^{\mathrm{T}}\big(\boldsymbol{T}_{,\dot{\boldsymbol{q}}}(\boldsymbol{q}_k, \boldsymbol{u}_k, t_k) + \boldsymbol{T}_{,\dot{\boldsymbol{q}}}(\boldsymbol{q}_{k+1}, \boldsymbol{u}_k, t_{k+1})\big)\,.\end{aligned} \tag{5}$$

Using $\boldsymbol{b} = \boldsymbol{T}_{,\boldsymbol{q}} + \boldsymbol{f} + \boldsymbol{W}\boldsymbol{\lambda}$, the first term of the variation of the kinetic energy and the external force contributions of (1) are discretized as

$$\begin{aligned}\sum_{k=1}^{N-1}\int_{t_k}^{t_{k+1}} \delta\boldsymbol{q}^{\mathrm{T}}\boldsymbol{b}(\boldsymbol{q},\dot{\boldsymbol{q}},t)\mathrm{d}t &\overset{(3)}{=} \sum_{k=1}^{N-1}\int_{t_k}^{t_{k+1}} \big((1-s_k)\delta\boldsymbol{q}_k + s_k\delta\boldsymbol{q}_{k+1}\big)^{\mathrm{T}}\boldsymbol{b}\big((1-s_k)\boldsymbol{q}_k + s_k\boldsymbol{q}_{k+1}, \boldsymbol{u}_k, t\big)\mathrm{d}t \\ &\overset{(4)}{=} \sum_{k=1}^{N-1}\frac{\Delta t}{2}\big(\delta\boldsymbol{q}_k^{\mathrm{T}}\boldsymbol{b}(\boldsymbol{q}_k, \boldsymbol{u}_k, t_k) + \delta\boldsymbol{q}_{k+1}^{\mathrm{T}}\boldsymbol{b}(\boldsymbol{q}_{k+1}, \boldsymbol{u}_k, t_{k+1})\big)\,.\end{aligned} \tag{6}$$

In what follows, the time dependency of the kinetic energy and the external force is dropped in the notation, as the time instant is always evaluated corresponding to the discrete coordinate, e.g. $\boldsymbol{f}(\boldsymbol{q}_k, \bullet) = \boldsymbol{f}(\boldsymbol{q}_k, \bullet, t_k)$. Using (5) and (6) in the virtual

action (1), we obtain the discrete virtual action

$$\begin{aligned}\delta A = \delta \boldsymbol{q}_1^{\mathrm{T}} \Bigg[-\frac{1}{2}\Big(T_{,\dot{\boldsymbol{q}}}\left(\boldsymbol{q}_1, \boldsymbol{u}_1\right) + T_{,\dot{\boldsymbol{q}}}\left(\boldsymbol{q}_2, \boldsymbol{u}_1\right)\Big) + \frac{\Delta t}{2}\Big(T_{,\boldsymbol{q}}\left(\boldsymbol{q}_1, \boldsymbol{u}_1\right) + \boldsymbol{f}(\boldsymbol{q}_1, \boldsymbol{u}_1) + \boldsymbol{W}_1 \boldsymbol{\lambda}_1 \Big) + \boldsymbol{W}_1 \boldsymbol{\Lambda}_1 + \boldsymbol{P}_0 \Bigg] \\ + \sum_{k=2}^{N-1} \delta \boldsymbol{q}_k^{\mathrm{T}} \Bigg[\frac{1}{2}\Big(T_{,\dot{\boldsymbol{q}}}\left(\boldsymbol{q}_{k-1}, \boldsymbol{u}_{k-1}\right) + T_{,\dot{\boldsymbol{q}}}\left(\boldsymbol{q}_k, \boldsymbol{u}_{k-1}\right) - T_{,\dot{\boldsymbol{q}}}\left(\boldsymbol{q}_k, \boldsymbol{u}_k\right) - T_{,\dot{\boldsymbol{q}}}\left(\boldsymbol{q}_{k+1}, \boldsymbol{u}_k\right)\Big) \\ + \frac{\Delta t}{2}\Big(T_{,\boldsymbol{q}}\left(\boldsymbol{q}_k, \boldsymbol{u}_{k-1}\right) + T_{,\boldsymbol{q}}\left(\boldsymbol{q}_k, \boldsymbol{u}_k\right) + \boldsymbol{f}(\boldsymbol{q}_k, \boldsymbol{u}_{k-1}) + \boldsymbol{f}(\boldsymbol{q}_k, \boldsymbol{u}_k) \Big) + \boldsymbol{W}_k(\Delta t \boldsymbol{\lambda}_k + \boldsymbol{\Lambda}_k) \Bigg] \\ + \delta \boldsymbol{q}_N^{\mathrm{T}} \Bigg[\frac{1}{2}\Big(T_{,\dot{\boldsymbol{q}}}\left(\boldsymbol{q}_{N-1}, \boldsymbol{u}_{N-1}\right) + T_{,\dot{\boldsymbol{q}}}\left(\boldsymbol{q}_N, \boldsymbol{u}_{N-1}\right) \Big) + \frac{\Delta t}{2}\Big(T_{,\boldsymbol{q}}\left(\boldsymbol{q}_N, \boldsymbol{u}_{N-1}\right) + \boldsymbol{f}(\boldsymbol{q}_N, \boldsymbol{u}_{N-1}) + \boldsymbol{W}_N \boldsymbol{\lambda}_N \Big) \\ + \boldsymbol{W}_N \boldsymbol{\Lambda}_N - \boldsymbol{P}_T \Bigg] .\end{aligned} \tag{7}$$

The principle of virtual action demands the virtual action (7) to vanish for all $\delta \boldsymbol{q}_k$ and induces the terms in the square brackets to be equal to zero. The vanishing of the first square bracket defines the first step of the numerical scheme, which is used to compute $\boldsymbol{q}_2$ from the initial position $\boldsymbol{q}_1$ and the initial velocity of the system. The initial velocity defines the intial impulsive force $\boldsymbol{P}_0$ through the boundary condition resulting from the principle of virtual action on (2), which is then used in the first step of the scheme. The second bracket defines the stepping equation for every other temporal node.

To specify the behavior of the unilateral constraints, we define the discrete percussion $\boldsymbol{P}_k = \Delta t \boldsymbol{\lambda}_k + \boldsymbol{\Lambda}_k$, which combines the effects of both the impulsive and the non-impulsive contact forces during a temporal element. We introduce the normal percussion $\boldsymbol{P}_{N,k}$ and the tangential percussion $\boldsymbol{P}_{T,k}$, such that $\boldsymbol{P}_k = (\boldsymbol{P}_{N,k}^{\mathrm{T}}\ \boldsymbol{P}_{T,k}^{\mathrm{T}})^{\mathrm{T}}$. Moreover, we introduce the kinematic quantities $\xi_{Ni,k} = \boldsymbol{w}_{N,i}^{\mathrm{T}}|_k(\boldsymbol{u}_{k+1} + \varepsilon_{Ni}\boldsymbol{u}_k)$ and $\boldsymbol{\xi}_{Ti,k} = \boldsymbol{w}_{T,i}^{\mathrm{T}}|_k(\boldsymbol{u}_{k+1} + \varepsilon_{Ti}\boldsymbol{u}_k)$ using the Newtonian restitution coefficient ε_{Ni} and ε_{Ti} for the i-th contact. This gives the framework to use the discrete constitutive contact law of Moreau [4] as done by [3], which takes into account Coulomb friction and a Newton type impact law. Finally, our stepping scheme is given by the stepping equation and the normal cone inclusions of the constitutive law, namely

$$\begin{aligned} 0 &= \frac{1}{2}\Big(T_{,\dot{\boldsymbol{q}}}\left(\boldsymbol{q}_{k-1}, \boldsymbol{u}_{k-1}\right) + T_{,\dot{\boldsymbol{q}}}\left(\boldsymbol{q}_k, \boldsymbol{u}_{k-1}\right) - T_{,\dot{\boldsymbol{q}}}\left(\boldsymbol{q}_k, \boldsymbol{u}_k\right) - T_{,\dot{\boldsymbol{q}}}\left(\boldsymbol{q}_{k+1}, \boldsymbol{u}_k\right)\Big) \\ &\quad + \frac{\Delta t}{2}\Big(T_{,\boldsymbol{q}}\left(\boldsymbol{q}_k, \boldsymbol{u}_{k-1}\right) + T_{,\boldsymbol{q}}\left(\boldsymbol{q}_k, \boldsymbol{u}_k\right) + \boldsymbol{f}(\boldsymbol{q}_k, \boldsymbol{u}_{k-1}) + \boldsymbol{f}(\boldsymbol{q}_k, \boldsymbol{u}_k) \Big) + \boldsymbol{W}_{N,k}\boldsymbol{P}_{N,k} + \boldsymbol{W}_{T,k}\boldsymbol{P}_{T,k} \\ \boldsymbol{u}_{k-1} &= (\boldsymbol{q}_k - \boldsymbol{q}_{k-1})/\Delta t\ , \qquad \boldsymbol{u}_k = (\boldsymbol{q}_{k+1} - \boldsymbol{q}_k)/\Delta t \\ -\xi_{Ni,k} &\in \mathcal{N}_{\mathbb{R}_0^+}(P_{Ni,k})\ , \qquad \forall i \in \mathcal{J} = \{i \,|\, g_i(\boldsymbol{q}_k) \le 0\} \\ -\boldsymbol{\xi}_{Ti,k} &\in \mathcal{N}_{C_T}(\boldsymbol{P}_{Ti,k})\ , \qquad \forall i \in \mathcal{J} = \{i \,|\, g_i(\boldsymbol{q}_k) \le 0\}\ , \end{aligned} \tag{8}$$

where C_T is the force reservoir of the percussion due to friction, e.g. $C_T = \{\boldsymbol{P}_T \mid ||\boldsymbol{P}_T|| \le \mu \boldsymbol{P}_N\}$ for isotropic Coulomb friction. For given coordinates $\boldsymbol{q}_{k-1}$ and $\boldsymbol{q}_k$, the subsequent coordinate $\boldsymbol{q}_{k+1}$ can be calculated by the stepping scheme (8). This gives iteratively the piecewise linear motion of the unilaterally constrained system $\mathcal{S}$. The normal cone inclusions in (8) can be reformulated as implicit proximal point equations, which can be solved at every time step by a fixed point iteration [3].

4 Numerical results

For mechanical systems with constant mass matrix and external forces not depending on the velocities, the proposed stepping scheme coincides with the well established stepping scheme of Moreau, cf. [3]. Most of the benchmark examples used for rigid multibody systems with multiple unilateral constraints and friction, such as the woodpecker toy [5], have constant mass matrix and constant external forces. Consequently, the presented integrator coincides with Moreau's scheme for the most common benchmark examples. To show the differences, we consider the spring pendulum of Fig. 1 having a non-constant mass matrix. The spring pendulum consists of a mass m connected to a pivot O by a spring with stiffness k and an undeformed length l_0. As generalized coordinates, the length $l(t)$ of the spring and the angle $\varphi(t)$ are chosen, i.e. $\boldsymbol{q}(t) = \big(l(t)\ \ \varphi(t)\big)^{\mathrm{T}}$. For $\varphi(t) = 0$ the pendulum is in contact with a vertical wall. The contact is characterized by the normal restitution coefficient ε_N and has no friction. The system is energy conserving during the contact free motion, as we assume that the spring pendulum is only subjected to gravity. Choosing the impact parameter $\varepsilon_N = 1$, no energy dissipates during the impacts and the motion of the spring pendulum preserves the energy E of the system. In Fig. 2 the relative energy error $e(t) = \frac{E(t)-E(0)}{E(0)}$ of the numerical solutions calculated by the proposed scheme (8) and Moreau's scheme are plotted over time. The energy error of Moreau's scheme becomes negative and very large in magnitude for the long-time simulation. We can see around 40% of energy dissipation after 250s of simulation time caused only by the numerical scheme. In contrast, the presented scheme

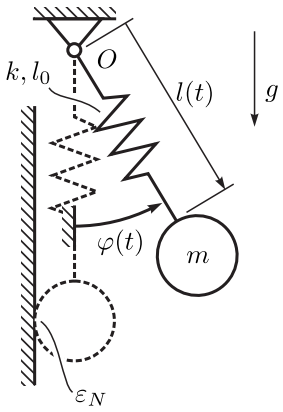

Fig. 1: The spring pendulum.

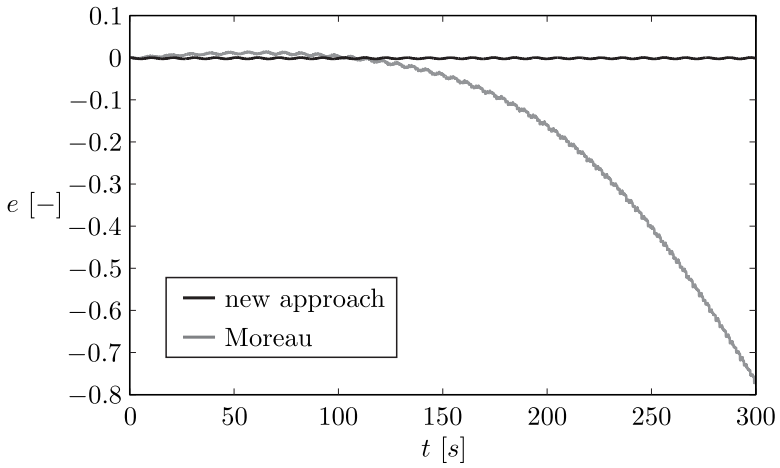

Fig. 2: Energy error e plotted over time t. Simulation parameters: $l_0 = 1$, $k = 100$, $g = 9.81$, $m = 1$, $\Delta t = 0.002$, $l(0) = 1.1$, $\varphi(0) = \pi/4$, $\dot{l}(0) = \dot{\varphi}(0) = 0$.

shows a stable long-time energy behavior with an energy error appearing to be bounded and oscillating around the zero error level with an amplitude of about 0.35%.

5 Conclusions

We presented a systematic approach to derive variational integrators for mechanical systems with frictional contacts. By combining the discretization of the virtual action with finite elements in time with the discrete contact law of Moreau, our scheme combines the qualities of the variational integrators and the contact law. The excellent long-time energy behavior shown for the spring pendulum is typical for variational integrators. On the other hand, our scheme can be used for systems with many frictional contacts, as granular media, and it can overcome accumulation points. Both properties are due to Moreau's contact law.

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