INTERNATIONAL JOURNAL FOR NUMERICAL METHODS IN ENGINEERING
Int. J. Numer. Meth. Engng 2017; **00**:1–21
Published online in Wiley Online Library (wileyonlinelibrary.com). DOI: 10.1002/nme

Time finite element based Moreau-type integrators

G. Capobianco*,† and S. R. Eugster

Institute for Nonlinear Mechanics, University of Stuttgart, Pfaffenwaldring 9, 70569 Stuttgart, Germany

SUMMARY

With the postulation of the principle of virtual action, we propose in this paper a variational framework for describing the dynamics of finite dimensional mechanical systems which contain frictional contact interactions. Together with the contact and impact laws formulated as normal cone inclusions, the principle of virtual action directly leads to the measure differential inclusions commonly used in the dynamics of nonsmooth mechanical systems. The discretization of the principle of virtual action in its strong and weak variational form by local finite elements in time provides a structured way to derive various time-stepping schemes. The constitutive laws for the impulsive and non-impulsive contact forces, i.e. the contact and impact laws, are treated on velocity-level by using a discrete contact law for the percussion increments in the sense of Moreau. Using linear shape functions and different quadrature rules, we obtain three different stepping schemes. Besides the well established Moreau time-stepping scheme, we can present two alternative integrators referred to as symmetric and variational Moreau-type stepping schemes. A suitable benchmark example shows the superiority of the newly proposed integrators in terms of energy conservation properties, accuracy and convergence.

Received ...

KEY WORDS: Multibody dynamics, time integration, time finite element method (TFEM), variational integrators, nonsmooth mechanics.

1. INTRODUCTION

This work is concerned with the numerical time-integration of the dynamical behavior of finite dimensional mechanical systems which contain frictional contact interactions. If such contact interactions are described by set-valued force laws, cf. [1], as for instance by unilateral constraints, the motion of such systems can be expected to not behave smoothly. In fact, an exact realization of such contact laws will lead to velocity jumps and undefined accelerations at collision time instants. As a consequence, the equations of motion, which require defined accelerations, fail to describe the motion at this very time instants. To obtain notwithstanding a well-defined description of the system, the equations of motion can be augmented by impact equations together with impact laws. Similarly to the contact laws, the impact laws have to be understood as constitutive laws and can be described by set-valued force laws. Typically, the equations of motion and the impact equations are combined into equality of measures. Together with the formulation of the contact and impact laws as set-valued force laws, this leads to a description of the dynamics of the nonsmooth mechanical system in the form of measure differential inclusions. Among the first to use this approach was J. J. Moreau, who also devised a numerical scheme to solve these measure differential inclusions [2]. We refer to this

*Correspondence to: Giuseppe Capobianco, Institute for Nonlinear Mechanics, University of Stuttgart, Pfaffenwaldring 9, 70569 Stuttgart, Germany
†E-mail: capobianco@inm.uni-stuttgart.de

well established scheme as *Moreau's time-stepping scheme*. Other discretizations of the measure differential inclusions have been developed, such as the modified Θ-method of Jean [3], the scheme of Paoli and Schatzman [4, 5] and the schemes of Stewart, Anitescu, Potra and Trinkle [6, 7, 8, 9]. We refer to [10, 11] for a more detailed overview of existing methods. Moreau's time-stepping scheme has many advantages. As an event-capturing algorithm, which does not solve for every single impact, it is well suited for many contact problems such as the simulation of granular media [12, 13, 14, 15, 16]. Furthermore, it can also overcome accumulation points, which are characterized as sequences of infinitely many impacts appearing in a finite time interval. In contrast, Moreau's scheme shows poor longterm energy behavior, is of low order and allows for contact penetration. These drawbacks have been addressed in several works. Using the concept of discrete derivatives by Gonzalez [17], Möller [18] presents a scheme which is similar to the one of Moreau but conserves the energy. Acary [19] and Studer [10] use various techniques to arrive at higher order schemes. The problem of contact penetration is addressed in [20, 21, 22, 13].

The discretization of a variational principle, such as Hamilton's law of varying action [23], with finite elements in time has proven to be an effective and structured way to derive integration schemes for smooth mechanical systems. The so derived schemes often exhibit good longterm energy behavior, see for example [24, 25]. As shown by Marsden and West [26], the time finite element discretization of Hamilton's law of varying action leads to the realm of discrete mechanics and variational integrators. These integrators are known to be symplectic and to show a good longterm energy behavior, cf. [26, 27]. The framework of discrete mechanics is used in [28] and [29] to derive integration schemes for nonsmooth mechanical systems. This is done by the use of a space-time formalism, where the action functional of Hamilton is also varied with respect to time allowing to impose a jump condition on the energy, which for the case of a mechanical system with only one contact corresponds to the choice of an impact law . While the algorithm of [28] belongs to the class of event-driven algorithms, [29] proposes an approach allowing for discontinuous trajectories. The same discontinuous behavior of the trajectories is assumed in [30], where the discretization of a variational formulation of the equality of measures with a discontinuous Galerkin approach in time is discussed. This leads then to Moreau's time-stepping scheme together with some higher order schemes.

Event-capturing algorithms coming from the discretization of the equality of measures perform robustly for many-contact problems and can overcome accumulation points. Furthermore, the discretization of variational principles leads to a well-structured way to derive integration schemes which often exhibit good longterm simulation behavior. In the present work, we want to show how to combine these advantages by applying continuous shape functions for the approximation of the systems trajectories. In Section 2, we propose with the principle of virtual action a variational principle which, for forces belonging to the class of special functions with locally bounded variations, contains the equality of measures. Furthermore, the contact and impact laws for frictional contacts are formulated as normal cone inclusions. Section 3 shows the discretization of the principle of virtual action, in its strong and weak variational form, with piecewise linear shape functions in time. Together with a certain choice of quadrature rules three different time-stepping schemes are obtained. The schemes are completed by the discretization of the contact and impact laws in accordance with Moreau's time-stepping scheme. The three schemes are summarized in Section 4 and evaluated in Section 5 for certain benchmark examples. Finally, conclusions are drawn in Section 6.

2. NONSMOOTH MECHANICAL SYSTEMS

In this section, we introduce the principle of virtual action for finite dimensional mechanical systems, which serves as starting point for the derivation of the integrators. Furthermore, we show that the principle of virtual action implies the equality of measures or, equivalently, the equations of motion and the impact equations. Finally, the constitutive laws describing the contacts are introduced.

DOI: 10.1002/nme

Consider a finite dimensional mechanical system $\mathcal{S}$, whose configuration can be described by a finite set of generalized coordinates $\mathbf{q} \in \mathbb{R}^n$. A motion of the system $\mathcal{S}$ is a map $\mathbf{q}\colon \mathcal{I} \to \mathbb{R}^n,\ t \mapsto \mathbf{q}(t)$, which associates to every time instant t in the time interval $\mathcal{I} = [t_s, t_f] \subseteq \mathbb{R}$ a set of generalized coordinates. The time instants t_s and t_f indicate the starting and the final time of the considered motion. Wherever defined, the velocity and acceleration of the system at t are $\dot{\mathbf{q}}(t)$ and $\ddot{\mathbf{q}}(t)$ respectively, where $\dot{(\bullet)} = \frac{\mathrm{d}}{\mathrm{d}t}(\bullet)$ denotes the derivative with respect to time. The velocities $\dot{\mathbf{q}} \in \mathrm{SLBV}(\mathbb{R};\mathbb{R}^n)$ are assumed to be special functions of locally bounded variation. The space $\mathrm{SLBV}(\mathbb{R};\mathbb{R}^n)$ is defined in [31] as the subspace of the space of functions with locally bounded variation $\mathrm{LBV}(\mathbb{R};\mathbb{R}^n)$ which do not have a Cantor part, i.e. which have at most countably infinitely many jump discontinuities. Thus, the differential measure $\mathrm{d}\dot{\mathbf{q}}$ can be decomposed into the sum of an absolutely continuous and a singular measure with respect to the Lebesgue measure $\mathrm{d}t$, cf. [32]. In order to explicitly write the decomposition of $\mathrm{d}\dot{\mathbf{q}}$, we define the atomic measure as a finite sum of Dirac point measures δ_{t_k} by introducing

$$\mathrm{d}\eta = \sum_k \mathrm{d}\delta_{t_k}\ , \quad \text{where} \int_{\mathcal{I}} \mathrm{d}\delta_{t_k} = \begin{cases} 1 & \text{if } t_k \in \mathcal{I} \\ 0 & \text{if } t_k \notin \mathcal{I} \end{cases}\ , \tag{1}$$

which by definition is singular with respect to $\mathrm{d}t$. This allows to write the differential measure of any special function with locally bounded variation $\mathbf{s} \in \mathrm{SLBV}(\mathbb{R};\mathbb{R}^n)$ as

$$\mathrm{d}\mathbf{s} = \dot{\mathbf{s}}(t)\,\mathrm{d}t + [\mathbf{s}(t^+) - \mathbf{s}(t^-)]\mathrm{d}\eta\ , \tag{2}$$

where the evaluation of $\mathbf{s}$ at t^- and t^+ denotes the left and right limit of $\mathbf{s}$ at t. In particular, we can write

$$\mathrm{d}\dot{\mathbf{q}} = \ddot{\mathbf{q}}(t)\,\mathrm{d}t + [\dot{\mathbf{q}}(t^+) - \dot{\mathbf{q}}(t^-)]\,\mathrm{d}\eta\ . \tag{3}$$

A variational family of the motion is a parametrization of motions $\hat{\mathbf{q}}(t,\varepsilon)$ which is smooth with respect to the parameter $\varepsilon \in \mathbb{R}$ and contains the actual motion for $\varepsilon = \varepsilon_0$, i.e. $\mathbf{q}(t) = \hat{\mathbf{q}}(t,\varepsilon_0)$. The virtual displacement of the system $\mathcal{S}$ at time t is then defined as

$$\delta\mathbf{q}(t) = \left.\frac{\partial \hat{\mathbf{q}}}{\partial \varepsilon}\right|_{(t,\varepsilon_0)}\ . \tag{4}$$

As a function of time, we assume $\delta\mathbf{q}$ to be smooth. The time derivative $(\delta\mathbf{q})\dot{} = \frac{\mathrm{d}(\delta\mathbf{q})}{\mathrm{d}t}$ of the virtual displacement corresponds to the variation of the velocity wherever the latter is defined[†], i.e. $(\delta\mathbf{q})\dot{} = \delta(\dot{\mathbf{q}})$ holds almost everywhere. While the inertia of the system $\mathcal{S}$ is given by the kinetic energy $T(\mathbf{q},\dot{\mathbf{q}},t)$, all remaining forces acting on $\mathcal{S}$ are introduced by the vector measure $\mathrm{d}\mathbf{F}$. As fundamental equation in dynamics, we postulate the principle of virtual action which demands the virtual action of all forces acting on the mechanical system $\mathcal{S}$ to vanish for all virtual displacements $\delta\mathbf{q}$, i.e.

$$\delta A = \int_{\mathcal{I}} \left[\delta T(\mathbf{q},\dot{\mathbf{q}},t)\,\mathrm{d}t + \delta\mathbf{q}^{\mathrm{T}}\mathrm{d}\mathbf{F}\right] = 0 \quad \forall \delta\mathbf{q}\ , \tag{5}$$

where $\delta T = \frac{\partial T}{\partial \mathbf{q}}\delta\mathbf{q} + \frac{\partial T}{\partial \dot{\mathbf{q}}}(\delta\mathbf{q})\dot{}$. Due to the preceding discussion that $(\delta\mathbf{q})\dot{} = \delta(\dot{\mathbf{q}})$ holds almost everywhere $(a.e.)$, the difference between δT used in (5) and the variation of the kinetic energy, given by $\frac{\partial T}{\partial \mathbf{q}}\delta\mathbf{q} + \frac{\partial T}{\partial \dot{\mathbf{q}}}\delta(\dot{\mathbf{q}})$, is Lebesgue negligible. Accordingly, this difference does not change the value of the definite integral in (5) and we will henceforth refer to δT as the variation of the kinetic energy.

As Lagrange did in the first place, we formulate the mechanical principle in the form of the necessary condition for an extremum of a functional in the context of the calculus of variations.

[†]Since the velocity $\dot{\mathbf{q}} \in \mathrm{SLBV}(\mathbb{R};\mathbb{R}^n)$, also the time derivative of $\hat{\mathbf{q}}$ are defined almost everywhere with respect to the Lebesgue measure $\mathrm{d}t$. Therefore we have $\dot{\mathbf{q}} = \left.\frac{\partial \hat{\mathbf{q}}}{\partial t}\right|_{\varepsilon=\varepsilon_0}$ $a.e.$, which implies that $\frac{\partial \hat{\mathbf{q}}}{\partial t}$ is a variational family for the velocity. Hence by Schwarz' Theorem, the relation $\delta(\dot{\mathbf{q}}) = \frac{\partial}{\partial \varepsilon}\left(\frac{\partial \hat{\mathbf{q}}}{\partial t}\right)\Big|_{\varepsilon=\varepsilon_0} = \frac{\partial}{\partial t}\left(\left.\frac{\partial \hat{\mathbf{q}}}{\partial \varepsilon}\right|_{\varepsilon=\varepsilon_0}\right) = (\delta\mathbf{q})\dot{}$ holds almost everywhere.

DOI: 10.1002/nme

Hellinger [33][‡] emphasizes the importance of the mechanical principle being only of the form of, and not acutally, a necessary condition of an extremum of a functional. Whether a functional exists, such that the principle of virtual action is the respective necessary condition, depends not only on the forces acting on the system but also on the boundary conditions. If the occurring forces can be deduced from a potential $V(\mathbf{q},t)$ by $\delta\mathbf{q}^{\mathrm{T}}\mathrm{d}\mathbf{F} = -\delta V(\mathbf{q},t)\,\mathrm{d}t$ and the initial and final configurations of the system are known, i.e. the virtual displacements vanish on the boundary of $\mathcal{I}$, such a functional does exist. It is the very action functional $A = \int_{\mathcal{I}}(T-V)\,\mathrm{d}t$ introduced by Hamilton [35]. The principle of virtual action then takes the form of Hamilton's principle [36, p. 98; 23, p. 124]. One could consider the principle of virtual action (5) also as the principle of virtual work formulated in space-time. However, as virtual work is a settled term, which denotes the virtual work formulated in space only, and (5) has a strong resemblance to Hamilton's law of varying action [35, p. 307; 37; 23, p. 124], the term "principle of virtual action" seems to be more appropriate. From a purely mathematical point of view, we accept with the principle of virtual action the idea of considering forces as distributions in the sense of L. Schwartz [38], which naturally includes impulsive forces. In this context, the principle of virtual action can be seen as the extension of Lagrange's equations of the second kind, where the time derivative of $\frac{\partial T}{\partial\dot{\mathbf{q}}}$ is formulated as a weak time derivative. This allows for a bigger class of solution functions, which contains also the nonsmooth behavior of a system.

We assume that the system $\mathcal{S}$ is restricted by n_c rheonomic geometric unilateral constraints, which are represented by the inequalities $g_i(\mathbf{q},t) \geq 0$ for $i = 1,\dots,n_c$. For the i^{th} contact, the gap function g_i is zero in case of contact, positive in case of separation and negative in case of penetration. In addition to the gap functions, for $i = 1,\dots,n_c$, the normal and tangential contact velocities $\gamma_{Ni} = \dot{g}_i$ *a.e.* and $\boldsymbol{\gamma}_{Ti} \in \mathbb{R}^2$, respectively, are introduced in order to fully describe the kinematics of each contact. For mechanical systems, these contact velocities are of the form

$$\gamma_{Ni}(\mathbf{q},\dot{\mathbf{q}},t) = \mathbf{w}_{Ni}(\mathbf{q},t)^{\mathrm{T}}\dot{\mathbf{q}} + \eta_{Ni}(\mathbf{q},t), \quad \text{and} \quad \boldsymbol{\gamma}_{Ti}(\mathbf{q},\dot{\mathbf{q}},t) = \mathbf{W}_{Ti}(\mathbf{q},t)^{\mathrm{T}}\dot{\mathbf{q}} + \boldsymbol{\eta}_{Ti}(\mathbf{q},t)\,, \tag{6}$$

where one recognizes the generalized force directions

$$\mathbf{w}_{Ni} = \left(\frac{\partial\gamma_{Ni}}{\partial\dot{\mathbf{q}}}\right)^{\mathrm{T}} = \left(\frac{\partial g_i}{\partial\mathbf{q}}\right)^{\mathrm{T}} \quad \text{and} \quad \mathbf{W}_{Ti} = \left(\frac{\partial\boldsymbol{\gamma}_{Ti}}{\partial\dot{\mathbf{q}}}\right)^{\mathrm{T}}\,, \tag{7}$$

which by $\mathbf{W} = (\mathbf{w}_{N1},\dots,\mathbf{w}_{Nn_c},\mathbf{W}_{T1},\dots,\mathbf{W}_{Tn_c})$ can be collected in a $n \times 3n_c$-matrix of generalized force directions. It is well known [39, 40] that in order to model hard unilateral constraints, one needs to allow impulsive forces to account for impacts whenever a contact closes. To do so, we assume an additive force decomposition

$$\mathrm{d}\mathbf{F} = \mathbf{W}\mathrm{d}\mathbf{P} + \mathrm{d}\tilde{\mathbf{F}} \tag{8}$$

where $\mathbf{W}\mathrm{d}\mathbf{P}$ and $\mathrm{d}\tilde{\mathbf{F}}$ denote the force measures of all contact and noncontact forces, respectively. Moreover, the contact force measure is determined by the matrix of generalized force directions $\mathbf{W}$ together with the associated measure to the percussion $\mathbf{P} \in \mathrm{SLBV}(\mathbb{R};\mathbb{R}^{3n_c})$. Since the percussion $\mathbf{P}$ is a special function with locally bounded variation, we can write the differential measure in accordance with (2) as

$$\mathrm{d}\mathbf{P} = \boldsymbol{\lambda}\,\mathrm{d}t + \boldsymbol{\Lambda}\,\mathrm{d}\eta\,, \tag{9}$$

where $\boldsymbol{\lambda}(t) = \dot{\mathbf{P}}(t) \in \mathbb{R}^{3n_c}$ are the nonimpulsive contact forces, used to model persistent closed contacts and friction, and $\boldsymbol{\Lambda}(t) = \mathbf{P}(t^+) - \mathbf{P}(t^-) \in \mathbb{R}^{3n_c}$ are impulsive forces used to account for impacts. The contact force vectors $\boldsymbol{\Lambda} = (\Lambda_{N1},\dots,\Lambda_{Nnc},\boldsymbol{\Lambda}_{T1}^{\mathrm{T}},\dots,\boldsymbol{\Lambda}_{Tnc}^{\mathrm{T}})^{\mathrm{T}}$ and $\boldsymbol{\lambda} = (\lambda_{N1},\dots,\lambda_{Nnc},\boldsymbol{\lambda}_{T1}^{\mathrm{T}},\dots,\boldsymbol{\lambda}_{Tnc}^{\mathrm{T}})^{\mathrm{T}}$ contain the impulsive and nonimpulsive contact forces in normal and tangential direction $\Lambda_{Ni},\lambda_{Ni}$ and $\boldsymbol{\Lambda}_{Ti},\boldsymbol{\lambda}_{Ti} \in \mathbb{R}^2$, respectively, for all individual contacts $i = 1,\dots,n_c$. We will further assume that, except for two impulsive forces $\bar{\mathbf{p}}_s$ and $\bar{\mathbf{p}}_f$ on the boundary of $\mathcal{I}$, no other impulsive forces act on the system. Accordingly, we can write the virtual

[‡] An English translation of the relevant part of [33] can be found in [34].

DOI: 10.1002/nme

action contributions of the noncontact forces as

$$\int_{\mathcal{I}} \delta\mathbf{q}^{\mathrm{T}} \mathrm{d}\tilde{\mathbf{F}} = \int_{\mathcal{I}} \big(-\delta V(\mathbf{q},t) + \delta\mathbf{q}^{\mathrm{T}}\mathbf{f}\big)\,\mathrm{d}t - \big[\delta\mathbf{q}^{\mathrm{T}}\bar{\mathbf{p}}\big]_{\partial\mathcal{I}}\,, \tag{10}$$

where the notation $\big[\delta\mathbf{q}^{\mathrm{T}}\bar{\mathbf{p}}\big]_{\partial\mathcal{I}} = -\delta\mathbf{q}(t_s)^{\mathrm{T}}\bar{\mathbf{p}}_s + \delta\mathbf{q}(t_f)^{\mathrm{T}}\bar{\mathbf{p}}_f$ has been introduced and in which one part of the forces are deduced from a potential $V(\mathbf{q},t)$ and the others are not. The Lagrangian $L(\mathbf{q},\dot{\mathbf{q}},t)$ of the system is defined as the difference between the kinetic energy and the potential, i.e. $L(\mathbf{q},\dot{\mathbf{q}},t) = T(\mathbf{q},\dot{\mathbf{q}},t) - V(\mathbf{q},t)$. Using the Lagrangian together with (8) and (10) in (5) gives the weak (with respect to time) variational form of the principle of virtual action

$$\begin{aligned}\delta A &= \int_{\mathcal{I}} \big[\delta L(\mathbf{q},\dot{\mathbf{q}},t)\,\mathrm{d}t + \delta\mathbf{q}^{\mathrm{T}}(\mathbf{f}\,\mathrm{d}t + \mathbf{W}\mathrm{d}\mathbf{P})\big] - \big[\delta\mathbf{q}^{\mathrm{T}}\bar{\mathbf{p}}\big]_{\partial\mathcal{I}} \\ &= \int_{\mathcal{I}} \left[(\delta\mathbf{q})^{\cdot\mathrm{T}} \left(\frac{\partial L}{\partial\dot{\mathbf{q}}}\right)^{\mathrm{T}} \mathrm{d}t + \delta\mathbf{q}^{\mathrm{T}} \left(\left(\frac{\partial L}{\partial\mathbf{q}}\right)^{\mathrm{T}} \mathrm{d}t + \mathbf{f}\,\mathrm{d}t + \mathbf{W}\mathrm{d}\mathbf{P}\right)\right] - \big[\delta\mathbf{q}^{\mathrm{T}}\bar{\mathbf{p}}\big]_{\partial\mathcal{I}} = 0 \quad \forall\delta\mathbf{q}\,.\end{aligned} \tag{11}$$

Using integration by parts for every time interval between two subsequent discontinuity points of a function $\mathbf{s} \in \mathrm{SLBV}(\mathbb{R};\mathbb{R}^n)$, one can show that

$$\begin{aligned}\int_{\mathcal{I}} (\delta\mathbf{q})^{\cdot\mathrm{T}}\mathbf{s}\,\mathrm{d}t &\overset{(1)}{=} -\int_{\mathcal{I}} \delta\mathbf{q}^{\mathrm{T}}\dot{\mathbf{s}}\,\mathrm{d}t - \int_{\mathcal{I}} \delta\mathbf{q}^{\mathrm{T}}[\mathbf{s}(t^+) - \mathbf{s}(t^-)]\mathrm{d}\eta + \big[\delta\mathbf{q}^{\mathrm{T}}\mathbf{s}\big]_{\partial\mathcal{I}} \\ &\overset{(2)}{=} -\int_{\mathcal{I}} \delta\mathbf{q}^{\mathrm{T}}\mathrm{d}\mathbf{s} + \big[\delta\mathbf{q}^{\mathrm{T}}\mathbf{s}\big]_{\partial\mathcal{I}}\,,\end{aligned} \tag{12}$$

where the boundary terms have been abbreviated by $[\delta\mathbf{q}^{\mathrm{T}}\mathbf{s}]_{\partial\mathcal{I}} = -\delta\mathbf{q}(t_s)^{\mathrm{T}}\mathbf{s}(t_s) + \delta\mathbf{q}(t_f)^{\mathrm{T}}\mathbf{s}(t_f)$. The derivative $\frac{\partial L}{\partial\dot{\mathbf{q}}}$ of the Lagrangian in (11) is evaluated along the motion and the velocity of the system. Hence, $\frac{\partial L}{\partial\dot{\mathbf{q}}}(\mathbf{q}(\bullet),\dot{\mathbf{q}}(\bullet),\bullet)$ is a special function of locally bounded variation in time and we can apply the integration by parts formula (12) to the principle of virtual action (11), which leads to the strong variational form of the principle of virtual action

$$\delta A = \int_{\mathcal{I}} \delta\mathbf{q}^{\mathrm{T}} \left[-\mathrm{d}\left(\frac{\partial L}{\partial\dot{\mathbf{q}}}\right)^{\mathrm{T}} + \left(\frac{\partial L}{\partial\mathbf{q}}\right)^{\mathrm{T}}\mathrm{d}t + \mathbf{f}\,\mathrm{d}t + \mathbf{W}\mathrm{d}\mathbf{P}\right] + \left[\delta\mathbf{q}^{\mathrm{T}}\left(\left(\frac{\partial L}{\partial\dot{\mathbf{q}}}\right)^{\mathrm{T}} - \bar{\mathbf{p}}\right)\right]_{\partial\mathcal{I}} = 0 \tag{13}$$

for all $\delta\mathbf{q}$. Together with the decompostion of the contact forces (9) and the identity (2), this can also be written in a more extended form as

$$\begin{aligned}\delta A = &\int_{\mathcal{I}} \delta\mathbf{q}^{\mathrm{T}} \left[-\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial\dot{\mathbf{q}}}\right)^{\mathrm{T}} + \left(\frac{\partial L}{\partial\mathbf{q}}\right)^{\mathrm{T}} + \mathbf{f} + \mathbf{W}\boldsymbol{\lambda}\right]\mathrm{d}t \\ &+ \int_{\mathcal{I}} \delta\mathbf{q}^{\mathrm{T}} \left[\left(\frac{\partial L}{\partial\dot{\mathbf{q}}}\right)^{\mathrm{T}}\Big|_{t^-} - \left(\frac{\partial L}{\partial\dot{\mathbf{q}}}\right)^{\mathrm{T}}\Big|_{t^+} + \mathbf{W}\boldsymbol{\Lambda}\right]\mathrm{d}\eta \\ &- \delta\mathbf{q}(t_s)^{\mathrm{T}} \left[\left(\frac{\partial L}{\partial\dot{\mathbf{q}}}\right)^{\mathrm{T}}\Big|_{t_s^+} - \bar{\mathbf{p}}_s\right] + \delta\mathbf{q}(t_f)^{\mathrm{T}} \left[\left(\frac{\partial L}{\partial\dot{\mathbf{q}}}\right)^{\mathrm{T}}\Big|_{t_f^-} - \bar{\mathbf{p}}_f\right] = 0 \quad \forall\delta\mathbf{q}\,.\end{aligned} \tag{14}$$

Since the virtual action δA has to vanish for all virtual displacements $\delta\mathbf{q}$, the terms in the square brackets of (13) and (14) have to vanish. From (13), this implies the equality of measures

$$\mathrm{d}\left(\frac{\partial L}{\partial\dot{\mathbf{q}}}\right)^{\mathrm{T}} = \left[\left(\frac{\partial L}{\partial\mathbf{q}}\right)^{\mathrm{T}} + \mathbf{f}\right]\mathrm{d}t + \mathbf{W}\mathrm{d}\mathbf{P}\,, \tag{15}$$

which are equivalent to the equations of motion in the form of Lagrange's equation of the second kind

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial\dot{\mathbf{q}}}\right)^{\mathrm{T}} - \left(\frac{\partial L}{\partial\mathbf{q}}\right)^{\mathrm{T}} = \mathbf{f} + \mathbf{W}\boldsymbol{\lambda}\,, \tag{16}$$

DOI: 10.1002/nme

together with the impact equations

$$\left(\frac{\partial L}{\partial \dot{\mathbf{q}}}\right)^{\mathrm{T}}\bigg|_{t^+} - \left(\frac{\partial L}{\partial \dot{\mathbf{q}}}\right)^{\mathrm{T}}\bigg|_{t^-} = \mathbf{W}\boldsymbol{\Lambda} \,. \tag{17}$$

Both evolution equations are completed by the two boundary conditions

$$\left(\frac{\partial L}{\partial \dot{\mathbf{q}}}\right)^{\mathrm{T}}\bigg|_{t_s^+} = \bar{\mathbf{p}}_s \qquad \text{and} \qquad \left(\frac{\partial L}{\partial \dot{\mathbf{q}}}\right)^{\mathrm{T}}\bigg|_{t_f^-} = \bar{\mathbf{p}}_f \,. \tag{18}$$

Therefore, the impulsive forces $\bar{\mathbf{p}}_s$ and $\bar{\mathbf{p}}_f$ give the generalized momentum of the system at the beginning and the end of the considered time interval, respectively. As in dynamics we are often interested in an initial value problem rather than in a boundary value problem, we can use $\bar{\mathbf{p}}_s$ to impose the initial condition on the generalized momentum, and therefore on the velocity, and leave $\bar{\mathbf{p}}_f$ free, allowing an arbitrary final velocity. Note that the equations of motion (16) just hold almost everywhere. The time instants on which they are not defined, are the impact time instants when $\boldsymbol{\Lambda} \neq 0$.

The kinetic energy of a general finite dimensional mechanical system is of the form

$$T(\mathbf{q}, \dot{\mathbf{q}}, t) = \frac{1}{2}\dot{\mathbf{q}}^{\mathrm{T}}\mathbf{M}(\mathbf{q}, t)\dot{\mathbf{q}} + \mathbf{a}(\mathbf{q}, t)^{\mathrm{T}}\dot{\mathbf{q}} + c(\mathbf{q}, t) \,, \tag{19}$$

where $\mathbf{M}(\mathbf{q}, t)$ is the symmetric positive definite mass matrix of the system, cf. [41, § 9.3]. The functions $\mathbf{M}$, $\mathbf{a}$ and c are assumed to be continuous and sufficiently smooth. Therefore, the generalized momentum, denoted by $\mathbf{p}$, takes the form

$$\mathbf{p}(\mathbf{q}, \dot{\mathbf{q}}, t) = \left(\frac{\partial L}{\partial \dot{\mathbf{q}}}\right)^{\mathrm{T}}(\mathbf{q}, \dot{\mathbf{q}}, t) = \left(\frac{\partial T}{\partial \dot{\mathbf{q}}}\right)^{\mathrm{T}}(\mathbf{q}, \dot{\mathbf{q}}, t) = \mathbf{M}(\mathbf{q}, t)\dot{\mathbf{q}} + \mathbf{a}(\mathbf{q}, t) \,, \tag{20}$$

as the potential $V(\mathbf{q}, t)$ does not depend on the velocity of the system. The associated differential measure with respect to time is

$$\mathrm{d}\mathbf{p} = \mathrm{d}\left(\frac{\partial L}{\partial \dot{\mathbf{q}}}\right)^{\mathrm{T}} \overset{(2)}{=} \left(\mathbf{M}\ddot{\mathbf{q}} + \dot{\mathbf{M}}\dot{\mathbf{q}} + \dot{\mathbf{a}}\right)\mathrm{d}t + \mathbf{M}(\dot{\mathbf{q}}^+ - \dot{\mathbf{q}}^-)\mathrm{d}\eta \overset{(3)}{=} \mathbf{M}\mathrm{d}\dot{\mathbf{q}} + \left(\dot{\mathbf{M}}\dot{\mathbf{q}} + \dot{\mathbf{a}}\right)\mathrm{d}t \,. \tag{21}$$

In order to keep the notation as short as possible, we introduce the force vectors

$$\mathbf{h}(\mathbf{q}, \dot{\mathbf{q}}, t) = \left(\frac{\partial L}{\partial \mathbf{q}}\right)^{\mathrm{T}}(\mathbf{q}, \dot{\mathbf{q}}, t) + \mathbf{f}(\mathbf{q}, \dot{\mathbf{q}}, t) - \dot{\mathbf{M}}(\mathbf{q}, \dot{\mathbf{q}}, t)\dot{\mathbf{q}} - \dot{\mathbf{a}}(\mathbf{q}, \dot{\mathbf{q}}, t) \,, \tag{22}$$

and

$$\mathbf{b}(\mathbf{q}, \dot{\mathbf{q}}, t) = \left(\frac{\partial L}{\partial \mathbf{q}}\right)^{\mathrm{T}}(\mathbf{q}, \dot{\mathbf{q}}, t) + \mathbf{f}(\mathbf{q}, \dot{\mathbf{q}}, t) \,. \tag{23}$$

Using the differential measure of the generalized momentum (21) together with (22), the equality of measures (15) can be restated in the form

$$\mathbf{M}(\mathbf{q}, t)\,\mathrm{d}\dot{\mathbf{q}} - \mathbf{h}(\mathbf{q}, \dot{\mathbf{q}}, t)\,\mathrm{d}t = \mathbf{W}(\mathbf{q}, t)\,\mathrm{d}\mathbf{P} \,, \tag{24}$$

which corresponds to Moreau's equation (7.4) in [2, p. 34] and which can also be found in various presentations on the dynamics of nonsmooth mechanical systems, cf. [3, 40, 42, 11] to name a few. Moreover, using (20) and (22), the equations of motion (16) can be written as

$$\mathbf{M}(\mathbf{q}, t)\,\ddot{\mathbf{q}} - \mathbf{h}(\mathbf{q}, \dot{\mathbf{q}}, t) = \mathbf{W}(\mathbf{q}, t)\,\boldsymbol{\lambda} \tag{25}$$

and, similarly, the impact equations as

$$\mathbf{M}(\mathbf{q}, t)\left(\dot{\mathbf{q}}(t^+) - \dot{\mathbf{q}}(t^-)\right) = \mathbf{W}(\mathbf{q}, t)\,\boldsymbol{\Lambda} \,. \tag{26}$$

DOI: 10.1002/nme

The equality of measure (24) together with the boundary conditions (18) are equivalent to the triplet consisting of the equations of motion (25), the impact equations (26) and the boundary conditions (18). Moreover, both these nonvariational characterizations of the motion of a mechanical system are equivalent to the principle of virtual action (11) and (13), respectively.

To complete the description of the frictional contacts, we specify the constitutive equations for the contact forces $\boldsymbol{\lambda}$ and $\boldsymbol{\Lambda}$ similarly to [10] for each individual contact $i = 1, \dots, n_c$. In normal direction to the contact plane we can formulate the impenetrability condition as the normal cone inclusion

$$-g_i \in \mathcal{N}_{\mathbb{R}_0^+}(\lambda_{Ni}) \quad \Leftrightarrow \quad g_i \geq 0,\ \lambda_{Ni} \geq 0,\ \lambda_{Ni}\, g_i = 0\ , \tag{27}$$

known as Signorini's condition [1]. For $g_i = 0$, the impulsive force Λ_{Ni} is specified by a Newton-type impact law

$$-\xi_{Ni} \in \mathcal{N}_{\mathbb{R}_0^+}(\Lambda_{Ni}) \quad \text{with} \quad \xi_{Ni} = \gamma_{Ni}^+ + e_{Ni}\gamma_{Ni}^-\ , \tag{28}$$

where we denote the restitution coefficient in normal direction by e_{Ni} and the pre- and post-impact velocities by $\gamma_{Ni}^- = \gamma_{Ni}(t^-)$ and $\gamma_{Ni}^+ = \gamma_{Ni}(t^+)$, respectively. For $g_i > 0$, when the contact is open, $\Lambda_{Ni} = 0$ is zero. We model the tangential contact forces $\boldsymbol{\lambda}_{Ti}$, i.e. friction forces in the contact plane, as Coulomb friction, which is described by

$$-\boldsymbol{\gamma}_{Ti} \in \mathcal{N}_{C_{Ti}(\lambda_{Ni})}(\boldsymbol{\lambda}_{Ti}) \tag{29}$$

where $C_{Ti}(\lambda_{Ni})$ specifies the set of possible friction forces, e.g. $C_{Ti}(\lambda_{Ni}) = \{\boldsymbol{\lambda}_{Ti} \in \mathbb{R}^2 |\ ||\boldsymbol{\lambda}_{Ti}|| \leq \mu_i \lambda_{Ni}\}$ for isotropic friction with friction coefficient μ_i. For closed contacts $g_i = 0$, we assume a Newton-type frictional impact law of the form

$$-\boldsymbol{\xi}_{Ti} \in \mathcal{N}_{C_{Ti}(\lambda_{Ni})}(\boldsymbol{\Lambda}_{Ti}) \quad \text{with} \quad \boldsymbol{\xi}_{Ti} = \boldsymbol{\gamma}_{Ti}^+ + e_{Ti}\boldsymbol{\gamma}_{Ti}^-\ , \tag{30}$$

where e_{Ti} denotes the restitution coefficient in tangential direction. As in normal direction, when the contact is open $g_i > 0$, there can be no impact and $\boldsymbol{\Lambda}_{Ti} = 0$ is accordingly set to zero. Reformulating (27) on velocity level as done in [1] and exploiting the cone structure of the constitutive laws, (27)–(30) can be combined to

$$-\xi_{Ni} \in \mathcal{N}_{\mathbb{R}_0^+}(\mathrm{d}P_{Ni}) \quad \text{and} \quad -\boldsymbol{\xi}_{Ti} \in \mathcal{N}_{C_{Ti}(\mathrm{d}P_{Ni})}(\mathrm{d}\mathbf{P}_{Ti}) \tag{31}$$

if $g_i = 0$. Otherwise the differentials of the percussions $\mathrm{d}P_{Ni}$ and $\mathrm{d}\mathbf{P}_{Ti}$ are set to zero. For a more detailed discussion about the constitutive contact laws and the combination to the formulation in terms of measures we refer to [10]. Furthermore, a didactic introduction to contact laws formulated as normal cone inclusions can be found in [43].

3. TIME FINITE ELEMENT DISCRETIZATION

In this section, we propose three different discretizations of the principle of virtual action. These discretizations differ by the choice whether the strong or the weak variational form is discretized and what quadrature rule is applied. While the discretization of the weak variational form can be understood as the Bubnov-Galerkin method, the discretization of the strong variational form corresponds to the weighted residual approach. To begin with, by introducing generic local shape functions in time, the infinite dimensional formulation of the principle of virtual action is reduced to a finite set of nonlinear equations. In a second step, we reduce the set of possible shape functions and assume the approximated motion to be piecewise linear. The choice of different quadrature rules for the integral over time then leads finally to the respective discretizations.

Let $(t_1 \leq \dots \leq t_N)$ be N time instants subdividing the time interval $\mathcal{I} = [t_s, t_f]$ into $n_{\mathrm{el}} = N - 1$ temporal elements $\Omega^e = [t_e, t_{e+1})$ indexed by $(\bullet)^e$ or $(\bullet)_e$, where $e = 1, \dots, n_{\mathrm{el}}$. The time interval $\Delta t^e = t_{e+1} - t_e$ denotes the temporal length of the element e. For every element e, let $\boldsymbol{\varphi}^e(s^e, \mathbf{z}^e)$ be the shape function of the element, which depends on the element parameter $s^e \in [0, 1]$ and the element coordinates $\mathbf{z}^e$. We assemble the element shape functions to a global shape function $\boldsymbol{\varphi}(t, \mathbf{z})$,

DOI: 10.1002/nme

which depends not only on time t but also on the collection $\mathbf{z}$ of all element coordinates $\mathbf{z}^e$. The global and local coordinates are related by some connectivity matrix $\mathbf{C}^e$, which extracts the local coordinates from the global coordinates by $\mathbf{z}^e = \mathbf{C}^e\mathbf{z}$. The approximation of the system's motion can then be considered as the constrained motion given by

$$\mathbf{q}(t) = \boldsymbol{\varphi}(t, \mathbf{z}) = \sum_{e=1}^{n_{\mathrm{el}}} \chi_{\Omega^e}(t)\ \boldsymbol{\varphi}^e(s^e(t), \mathbf{z}^e) \quad \text{with} \quad s^e(t) = \frac{t - t_e}{\Delta t^e} \quad \text{for} \quad t \in \Omega^e\ , \tag{32}$$

where $\chi_{\Omega^e}(t)$ is the characteristic function on the set Ω^e. The characteristic function is equal to one if $t \in \Omega^e$ and zero otherwise. Considering a smooth variational family of element coordinates $\hat{\mathbf{z}}^e(\varepsilon)$, containing the actual coordinates in the form $\hat{\mathbf{z}}^e(\varepsilon_0) = \mathbf{z}^e$, the variation of the element coordinate is

$$\delta\mathbf{z}^e = \left.\frac{\partial \hat{\mathbf{z}}^e}{\partial \varepsilon}\right|_{\varepsilon_0}\ . \tag{33}$$

Thus by equation (32), the variational family $\hat{\mathbf{z}}^e$ induces a variational family of motions $\hat{\mathbf{q}}(t, \varepsilon) = \boldsymbol{\varphi}^e(s^e(t), \hat{\mathbf{z}}^e(\varepsilon))$ for $t \in \Omega^e$, which using (4) gives the virtual displacement

$$\delta\mathbf{q}(t) = \left.\frac{\partial \boldsymbol{\varphi}^e}{\partial \mathbf{z}^e}\right|_{(s^e(t), \mathbf{z}^e)} \left.\frac{\partial \hat{\mathbf{z}}^e}{\partial \varepsilon}\right|_{\varepsilon_0} \overset{(33)}{=} \mathbf{N}^e(s^e(t), \mathbf{z}^e)\, \delta\mathbf{z}^e, \quad t \in \Omega^e\ , \tag{34}$$

where we have introduced the function $\mathbf{N}^e = \frac{\partial \boldsymbol{\varphi}^e}{\partial \mathbf{z}^e}$. By construction, the induced virtual displacement (34) is admissible with respect to the constraint (32). We constrain the motion in the weak variational form of the principle of virtual action (11) to the special form (32) by means of ideal constraint forces, which by the principle of d'Alembert–Lagrange have no contribution to the virtual action if the kinematics is chosen admissible to the constraint. Therefore, the weak variational form of the principle of virtual action (11) for admissible virtual displacements (34) together with (20) and (23) becomes

$$\delta A = \sum_{e=1}^{n_{\mathrm{el}}} \int_{\Omega^e} \left[\delta\mathbf{z}^{e\,\mathrm{T}} \dot{\mathbf{N}}^{e\,\mathrm{T}} \mathbf{p}\, \mathrm{d}t + \delta\mathbf{z}^{e\,\mathrm{T}} \mathbf{N}^{e\,\mathrm{T}} (\mathbf{b}\, \mathrm{d}t + \mathbf{W} \mathrm{d}\mathbf{P})\right] - \left[\delta\mathbf{z}^{e\,\mathrm{T}} \mathbf{N}^{e\,\mathrm{T}} \bar{\mathbf{p}}\right]_{\partial\mathcal{I}} = 0 \tag{35}$$

for all $\delta\mathbf{z}^e$ and all e, where the boundary terms are

$$\left[\delta\mathbf{z}^{e\,\mathrm{T}} \mathbf{N}^{e\,\mathrm{T}} \bar{\mathbf{p}}\right]_{\partial\mathcal{I}} = -(\mathbf{N}^1 \delta\mathbf{z}^1)^{\mathrm{T}}\Big|_{t=t_s} \bar{\mathbf{p}}_s + (\mathbf{N}^{n_{\mathrm{el}}} \delta\mathbf{z}^{n_{\mathrm{el}}})^{\mathrm{T}}\Big|_{t=t_f} \bar{\mathbf{p}}_f\ . \tag{36}$$

In equation (35), all quantities are evaluated along the constrained motion (32). The generalized momentum (20) within the element e is for instance given by $\mathbf{p}\big(\boldsymbol{\varphi}^e(s^e(t), \mathbf{z}^e), \dot{\boldsymbol{\varphi}}^e(s^e(t), \mathbf{z}^e), t\big)$.

In the same way, we constrain the strong variational form of the principle of virtual action (13) to the motion (32). Using (20) and the equivalence between (15) and (24) to rewrite the integrand in (13), leads to

$$\delta A = \sum_{e=1}^{n_{\mathrm{el}}} \int_{\Omega^e} \delta\mathbf{z}^{e\,\mathrm{T}} \mathbf{N}^{e\,\mathrm{T}} \left[-\mathbf{M}\, \mathrm{d}\dot{\boldsymbol{\varphi}} + \mathbf{h}\, \mathrm{d}t + \mathbf{W}\, \mathrm{d}\mathbf{P}\right] + \left[\delta\mathbf{z}^{e\,\mathrm{T}} \mathbf{N}^{e\,\mathrm{T}} \big(\mathbf{p} - \bar{\mathbf{p}}\big)\right]_{\partial\mathcal{I}} = 0 \tag{37}$$

for all $\delta\mathbf{z}^e$ and all e, where again all quantities are evaluated along the constrained motion (32). Choosing some quadrature rule in (35) or (37), these principles lead to algebraic systems of equations, which together with the constitutive laws for the forces determine $\mathbf{z}^e$ for all elements e. These element coordinates then give an approximation of the motion of the system $\mathcal{S}$ by (32). If one is interested in the solution of an initial value problem, most of the time, the algebraic system of equations can be rewritten as a stepping scheme, meaning that the equations can be decoupled such that the motion can be computed sequentially for each element starting from the first. In this case it is not needed to construct the whole algebraic system of equations and then extract the stepping

DOI: 10.1002/nme

scheme, as done e.g. in [44]. However, the decoupling can directly be recognized in the variational formulation as we will see below.

To derive the three integration schemes, we choose a piecewise linear motion and equidistant temporal nodes implying $\Delta t^e = \Delta t \; \forall e$ for some constant time step Δt. The nodal coordinates $\mathbf{q}_k \approx \mathbf{q}(t_k)$ are introduced such that they approximate the generalized coordinates of the system at the temporal nodes t_k. The piecewise linear motion is then given by the linear interpolation between two neighboring nodal coordinates implying the element shape function

$$\boldsymbol{\varphi}^e(s^e, \mathbf{z}^e) = (1 - s^e)\, \mathbf{q}_e + s^e\, \mathbf{q}_{e+1} = \underbrace{\begin{pmatrix}(1-s^e)\mathbf{I} & s^e\mathbf{I}\end{pmatrix}}_{\mathbf{N}(s^e)} \mathbf{z}^e, \quad \text{where} \quad \mathbf{z}^e = \begin{pmatrix}\mathbf{q}_e \\ \mathbf{q}_{e+1}\end{pmatrix} \tag{38}$$

and $\mathbf{I} \in \mathbb{R}^{n\times n}$ is the identity matrix. With these linear shape functions, the constrained motion (32) in the interior of each temporal element has constant velocity within an element, which we denote by $\mathbf{u}_e$, and zero acceleration, i.e. for $t \in \operatorname{int}(\Omega^e) = (t_e, t_{e+1})$

$$\dot{\mathbf{q}}(t) = \dot{\boldsymbol{\varphi}}^e(s^e(t), \mathbf{z}_e) = \frac{1}{\Delta t}(\mathbf{q}_{e+1} - \mathbf{q}_e) = \mathbf{u}_e \quad \text{and} \quad \ddot{\mathbf{q}}(t) = \ddot{\boldsymbol{\varphi}}^e(s^e(t), \mathbf{z}_e) = 0\,. \tag{39}$$

Moreover, the shape function (38) induces by equation (34) the admissible virtual displacements

$$\delta\mathbf{q}(t) = (1 - s^e(t))\, \delta\mathbf{q}_e + s^e(t)\, \delta\mathbf{q}_{e+1} \quad \text{and} \quad (\delta\mathbf{q})\dot{}\,(t) = \frac{1}{\Delta t}(\delta\mathbf{q}_{e+1} - \delta\mathbf{q}_e) \tag{40}$$

for $t \in \Omega^e$ and $t \in \operatorname{int}(\Omega^e)$, respectively. The differential measure $\mathrm{d}\dot{\boldsymbol{\varphi}}$ of the velocity of the constrained motion (32) contains only jump parts, as the acceleration is zero almost everywhere. By equation (39) the velocity jumps occur at the element nodes t_e for $e = 2, \ldots, N-1$. Furthermore, it follows that the left limit of the velocity at t_e is $\mathbf{u}_{e-1}$ and the right limit is $\mathbf{u}_e$. The differential measure of the motion then takes the form

$$\mathrm{d}\dot{\mathbf{q}} \overset{(32)}{=} \mathrm{d}\dot{\boldsymbol{\varphi}} \overset{(2)}{=} \sum_{e=2}^{N-1} (\mathbf{u}_e - \mathbf{u}_{e-1})\, \mathrm{d}\delta_{t_e}\,. \tag{41}$$

Using (38)–(41), the strong variational form of the principle of virtual action (37) leads to

$$\begin{aligned}\delta A = \sum_{e=1}^{n_{\mathrm{el}}} \begin{pmatrix}\delta\mathbf{q}_e \\ \delta\mathbf{q}_{e+1}\end{pmatrix}^{\mathrm{T}} \int_{\Omega^e} \mathbf{N}^{e\,\mathrm{T}} [\mathbf{h}\,\mathrm{d}t + \mathbf{W}\,\mathrm{d}\mathbf{P}] - \sum_{e=2}^{N-1} \delta\mathbf{q}_e^{\mathrm{T}} \mathbf{M}(\mathbf{q}_e, t_e)\big(\mathbf{u}_e - \mathbf{u}_{e-1}\big) \\ - \delta\mathbf{q}_1^{\mathrm{T}}\big[\mathbf{p}(\mathbf{q}_1, \mathbf{u}_1, t_1) - \bar{\mathbf{p}}_s\big] + \delta\mathbf{q}_N^{\mathrm{T}}\big[\mathbf{p}(\mathbf{q}_N, \mathbf{u}_{N-1}, t_N) - \bar{\mathbf{p}}_f\big] = 0 \quad \forall\delta\mathbf{q}_k \; \forall k\,.\end{aligned} \tag{42}$$

We approximate the integral over $\Omega^e = [t_e, t_{e+1})$ by evaluating the integrand at the upper bound of the time interval and multiplying it with the length of the temporal element Δt, i.e.

$$\int_{\Omega^e} \mathbf{N}^{e\,\mathrm{T}} [\mathbf{h}\,\mathrm{d}t + \mathbf{W}\,\mathrm{d}\mathbf{P}] \approx \begin{pmatrix}0 \\ \mathbf{I}\end{pmatrix} \big[\mathbf{h}(\mathbf{q}_{e+1}, \mathbf{u}_e, t_{e+1})\Delta t + \mathbf{W}(\mathbf{q}_{e+1}, t_{e+1})\mathbf{P}_{e+1}\big]\,, \tag{43}$$

where we have introduced the notation $\mathbf{P}_e = \Delta t\boldsymbol{\lambda}(t_e) + \boldsymbol{\Lambda}(t_e)$. Using this quadrature rule in (42) and rearranging the sum, we obtain

$$\begin{aligned}\delta A = \sum_{k=2}^{N-1} \delta\mathbf{q}_k^{\mathrm{T}} \Big[- \mathbf{M}(\mathbf{q}_k, t_k)\big(\mathbf{u}_k - \mathbf{u}_{k-1}\big) + \mathbf{h}(\mathbf{q}_k, \mathbf{u}_{k-1}, t_k)\Delta t + \mathbf{W}(\mathbf{q}_k, t_k)\mathbf{P}_k \Big] \\ + \delta\mathbf{q}_N^{\mathrm{T}}\big[\mathbf{p}(\mathbf{q}_N, \mathbf{u}_{N-1}, t_N) + \mathbf{h}(\mathbf{q}_N, \mathbf{u}_{N-1}, t_N)\Delta t + \mathbf{W}(\mathbf{q}_N, t_N)\mathbf{P}_N - \bar{\mathbf{p}}_f\big] \\ - \delta\mathbf{q}_1^{\mathrm{T}}\Big[\mathbf{p}(\mathbf{q}_1, \mathbf{u}_1, t_1) - \bar{\mathbf{p}}_s\Big] = 0 \quad \forall\delta\mathbf{q}_k \; \forall k\,.\end{aligned} \tag{44}$$

A necessary condition for the virtual action in (44) to vanish is that

$$-\mathbf{M}(\mathbf{q}_k, t_k)\big(\mathbf{u}_k - \mathbf{u}_{k-1}\big) + \mathbf{h}(\mathbf{q}_k, \mathbf{u}_{k-1}, t_k)\Delta t + \mathbf{W}(\mathbf{q}_k, t_k)\mathbf{P}_k = 0 \tag{45}$$

DOI: 10.1002/nme

for $k = 2, \dots, N-1$, which together with the definition of $\mathbf{u}_k$ in (39) defines a stepping scheme. Introducing constitutive laws for the forces, this scheme allows to calculate the generalized coordinates $\mathbf{q}_{k+1}$ from known coordinates $\mathbf{q}_{k-1}$ and $\mathbf{q}_k$ at previous time instants. Combining this scheme with the discrete contact law of Moreau, which we introduce below, yields Moreau's time-stepping scheme, cf. [2, 45, 42, 11]. As also the other terms in the square brackets of the principle of virtual action (44) have to vanish, the first step ($k = 1$) of the scheme is given by

$$\mathbf{p}(\mathbf{q}_1, \mathbf{u}_1, t_1) - \bar{\mathbf{p}}_s = 0 \,. \tag{46}$$

This, by equation (18), implies that the velocity of the first element $\mathbf{u}_1$ can be set equal to the initial velocity of the system, instead of computing the first step.

To obtain a different scheme, the trapezoidal rule is used for the integral (43), leading to the approximation of the integral

$$\int_{\Omega^e} \mathbf{N}^{e\,\mathrm{T}} \left[\mathbf{h}\,\mathrm{d}t + \mathbf{W}\,\mathrm{d}\mathbf{P}\right] \approx \frac{1}{2} \begin{pmatrix} \mathbf{h}(\mathbf{q}_e, \mathbf{u}_e, t_e)\Delta t + \mathbf{W}(\mathbf{q}_e, t_e)\mathbf{P}_e \\ \mathbf{h}(\mathbf{q}_{e+1}, \mathbf{u}_e, t_{e+1})\Delta t + \mathbf{W}(\mathbf{q}_{e+1}, t_{e+1})\mathbf{P}_{e+1} \end{pmatrix} \,. \tag{47}$$

With this quadrature rule, the principle of virtual action (42) has the form

$$\begin{aligned} \delta A = & \\ & \sum_{k=2}^{N-1} \delta\mathbf{q}_k^{\mathrm{T}} \left[-\mathbf{M}(\mathbf{q}_k, t_k)\big(\mathbf{u}_k - \mathbf{u}_{k-1}\big) + \frac{1}{2}\Big(\mathbf{h}(\mathbf{q}_k, \mathbf{u}_{k-1}, t_k) + \mathbf{h}(\mathbf{q}_k, \mathbf{u}_k, t_k)\Big)\Delta t + \mathbf{W}(\mathbf{q}_k, t_k)\mathbf{P}_k \right] \\ & - \delta\mathbf{q}_1^{\mathrm{T}} \left[\mathbf{p}(\mathbf{q}_1, \mathbf{u}_1, t_1) - \frac{1}{2}\Big(\mathbf{h}(\mathbf{q}_1, \mathbf{u}_1, t_1)\Delta t + \mathbf{W}(\mathbf{q}_1, t_1)\mathbf{P}_1\Big) - \bar{\mathbf{p}}_s \right] \\ & + \delta\mathbf{q}_N^{\mathrm{T}} \left[\mathbf{p}(\mathbf{q}_N, \mathbf{u}_{N-1}, t_N) + \frac{1}{2}\Big(\mathbf{h}(\mathbf{q}_N, \mathbf{u}_{N-1}, t_N)\Delta t + \mathbf{W}(\mathbf{q}_N, t_N)\mathbf{P}_N\Big) - \bar{\mathbf{p}}_f \right] = 0 \quad \forall \delta\mathbf{q}_k \; \forall k \,. \end{aligned} \tag{48}$$

Once more, a stepping scheme can be extracted form the principle of virtual action as a necessary condition for the virtual action to vanish. The resulting symmetric stepping scheme

$$-\mathbf{M}(\mathbf{q}_k, t_k)\big(\mathbf{u}_k - \mathbf{u}_{k-1}\big) + \frac{1}{2}\Big(\mathbf{h}(\mathbf{q}_k, \mathbf{u}_{k-1}, t_k) + \mathbf{h}(\mathbf{q}_k, \mathbf{u}_k, t_k)\Big)\Delta t + \mathbf{W}(\mathbf{q}_k, t_k)\mathbf{P}_k = 0 \,, \tag{49}$$

together with the discrete contact law of Moreau, leads to a stepping scheme for mechanical systems with frictional contacts, which we call *symmetric Moreau-type time-stepping scheme*. The first step of the scheme is given by

$$\mathbf{p}(\mathbf{q}_1, \mathbf{u}_1, t_1) - \frac{1}{2}\Big(\mathbf{h}(\mathbf{q}_1, \mathbf{u}_1, t_1)\Delta t + \mathbf{W}(\mathbf{q}_1, t_1)\mathbf{P}_1\Big) - \bar{\mathbf{p}}_s = 0 \,, \tag{50}$$

which is also a necessary condition for a vanishing virtual action in (48). The quantity $\bar{\mathbf{p}}_s$ can be used to impose the initial condition for the velocity on the discretized motion. In fact, equation (18) links $\bar{\mathbf{p}}_s$ to the initial coordinate and velocity of the system. This is the most natural way to impose the initial condition. One may be tempted to set $\mathbf{u}_1$ equal to the initial velocity, but this leads to a bad approximation of the initial condition, especially for big time steps.

The third stepping scheme is derived by the discretization of the weak variational form of the virtual action (35). Therefore, we use (38)–(40) in (35) leading to the principle of virtual action for the piecewise linear motion. We approximate the arising integral by the trapezoidal rule, which gives the approximations

$$\int_{\Omega^e} \dot{\mathbf{N}}^{e\,\mathrm{T}} \mathbf{p}\,\mathrm{d}t \approx \frac{1}{2} \begin{pmatrix} -\mathbf{I} \\ \mathbf{I} \end{pmatrix} \big(\mathbf{p}(\mathbf{q}_e, \mathbf{u}_e, t_e) + \mathbf{p}(\mathbf{q}_{e+1}, \mathbf{u}_e, t_{e+1})\big) \tag{51}$$

and

$$\int_{\Omega^e} \mathbf{N}^{e\,\mathrm{T}} \left[\mathbf{b}\,\mathrm{d}t + \mathbf{W}\,\mathrm{d}\mathbf{P}\right] \approx \frac{1}{2} \begin{pmatrix} \mathbf{b}(\mathbf{q}_e, \mathbf{u}_e, t_e)\Delta t + \mathbf{W}(\mathbf{q}_e, t_e)\mathbf{P}_e \\ \mathbf{b}(\mathbf{q}_{e+1}, \mathbf{u}_e, t_{e+1})\Delta t + \mathbf{W}(\mathbf{q}_{e+1}, t_{e+1})\mathbf{P}_{e+1} \end{pmatrix} \,. \tag{52}$$

DOI: 10.1002/nme

Using these approximations in (35) and rearranging the summation leads to the principle of virtual action

$$\begin{aligned}
\delta A = \\
&\sum_{k=2}^{N-1} \delta\mathbf{q}_k^{\mathrm{T}} \Bigg[\frac{1}{2} \Big(-\mathbf{p}(\mathbf{q}_k,\mathbf{u}_k,t_k) - \mathbf{p}(\mathbf{q}_{k+1},\mathbf{u}_k,t_{k+1}) + \mathbf{p}(\mathbf{q}_{k-1},\mathbf{u}_{k-1},t_{k-1}) + \mathbf{p}(\mathbf{q}_k,\mathbf{u}_{k-1},t_k) \Big) \\
&\qquad + \frac{1}{2} \Big(\mathbf{b}(\mathbf{q}_k,\mathbf{u}_{k-1},t_k) + \mathbf{b}(\mathbf{q}_k,\mathbf{u}_k,t_k) \Big) \Delta t + \mathbf{W}(\mathbf{q}_k,t_k)\mathbf{P}_k \Bigg] \\
&- \delta\mathbf{q}_1^{\mathrm{T}} \Bigg[\frac{1}{2} \Big(\mathbf{p}(\mathbf{q}_1,\mathbf{u}_1,t_1) + \mathbf{p}(\mathbf{q}_2,\mathbf{u}_1,t_2) - \mathbf{b}(\mathbf{q}_1,\mathbf{u}_1,t_1)\Delta t - \mathbf{W}(\mathbf{q}_1,t_1)\mathbf{P}_1 \Big) - \bar{\mathbf{p}}_s \Bigg] \\
&+ \delta\mathbf{q}_N^{\mathrm{T}} \Bigg[\frac{1}{2} \Big(\mathbf{p}(\mathbf{q}_{N-1},\mathbf{u}_{N-1},t_{N-1}) + \mathbf{p}(\mathbf{q}_N,\mathbf{u}_{N-1},t_N) \Big) \\
&\qquad + \frac{1}{2} \Big(\mathbf{b}(\mathbf{q}_N,\mathbf{u}_{N-1},t_N)\Delta t + \mathbf{W}(\mathbf{q}_N,t_N)\mathbf{P}_N \Big) - \bar{\mathbf{p}}_f \Bigg] = 0 \quad \forall \delta\mathbf{q}_k \; \forall k \; .
\end{aligned} \tag{53}$$

As the virtual action has to vanish for all virtual displacements $\delta\mathbf{q}_k$, the terms in the square brackets have to vanish. This implies the *variational Moreau-type time-stepping scheme*, which has already been proposed by the authors in [46],

$$\begin{aligned}
0 = &\Bigg[\frac{1}{2} \Big(-\mathbf{p}(\mathbf{q}_k,\mathbf{u}_k,t_k) - \mathbf{p}(\mathbf{q}_{k+1},\mathbf{u}_k,t_{k+1}) + \mathbf{p}(\mathbf{q}_{k-1},\mathbf{u}_{k-1},t_{k-1}) + \mathbf{p}(\mathbf{q}_k,\mathbf{u}_{k-1},t_k) \Big) \\
&+ \frac{1}{2} \Big(\mathbf{b}(\mathbf{q}_k,\mathbf{u}_{k-1},t_k) + \mathbf{b}(\mathbf{q}_k,\mathbf{u}_k,t_k) \Big) \Delta t + \mathbf{W}(\mathbf{q}_k,t_k)\mathbf{P}_k \Bigg]
\end{aligned} \tag{54}$$

for $k > 1$ and the first step

$$0 = \frac{1}{2} \Big(\mathbf{p}(\mathbf{q}_1,\mathbf{u}_1,t_1) + \mathbf{p}(\mathbf{q}_2,\mathbf{u}_1,t_2) - \mathbf{b}(\mathbf{q}_1,\mathbf{u}_1,t_1)\Delta t - \mathbf{W}(\mathbf{q}_1,t_1)\mathbf{P}_1 \Big) - \bar{\mathbf{p}}_s \; . \tag{55}$$

For the discretization of the contact laws (31) we choose the discrete contact law used in Moreau's stepping scheme, cf. [10, p. 76]. For both the normal and tangential direction of the contact i at the temporal node t_k, the quantities $\boldsymbol{\xi}$ defined in (28) and (30) are

$$\begin{aligned}
\xi_{Ni,k}(\mathbf{q}_k,\mathbf{u}_{k-1},\mathbf{u}_k,t_k) &= \gamma_{Ni}(\mathbf{q}_k,\mathbf{u}_k,t_k) + e_{Ni}\,\gamma_{Ni}(\mathbf{q}_k,\mathbf{u}_{k-1},t_k) \\
\boldsymbol{\xi}_{Ti,k}(\mathbf{q}_k,\mathbf{u}_{k-1},\mathbf{u}_k,t_k) &= \boldsymbol{\gamma}_{Ti}(\mathbf{q}_k,\mathbf{u}_k,t_k) + e_{Ti}\,\boldsymbol{\gamma}_{Ti}(\mathbf{q}_k,\mathbf{u}_{k-1},t_k) \; ,
\end{aligned} \tag{56}$$

as due to the piecewise linear shape function (38) the pre- and post-impact velocities are $\gamma_{Ni}^- = \gamma_{Ni}(\mathbf{q}_k,\mathbf{u}_{k-1},t_k)$ and $\gamma_{Ni}^+ = \gamma_{Ni}(\mathbf{q}_k,\mathbf{u}_k,t_k)$, respectively, and likewise for the tangential direction. We use this discretization of the contact kinematics to introduce the discrete contact laws

$$-\xi_{Ni,k} \in \mathcal{N}_{\mathbb{R}_0^+}(P_{Ni,k}) \quad \text{and} \quad -\boldsymbol{\xi}_{Ti,k} \in \mathcal{N}_{C_{Ti}(P_{Ni,k})}(\mathbf{P}_{Ti,k}) \; , \tag{57}$$

which hold whenever $g_i(\mathbf{q}_k) \leq 0$. Otherwise the percussion increments $P_{Ni,k}$ and $\mathbf{P}_{Ti,k}$ are set to zero.

4. MOREAU-TYPE INTEGRATORS

In the previous section, we derived three different schemes for mechanical systems with frictional contacts. In this section we restate the course of action for the schemes. We assume that the initial conditions are $\mathbf{q}(t_s) = \mathbf{q}_s$ and $\dot{\mathbf{q}}(t_s) = \mathbf{u}_s$. Using these initial conditions, the initial impulsive force $\bar{\mathbf{p}}_s$ can be calculated from (18). The pair consisting of $\mathbf{q}_s$ and $\bar{\mathbf{p}}_s$ is used to impose the initial conditions on the discretized motion within the first step.

DOI: 10.1002/nme

4.1. Moreau's time-stepping scheme [10]

1. *First step ($k=1$).* Set $\mathbf{q}_1 = \mathbf{q}_s$ and solve (46) for $\mathbf{q}_2$, i.e. solve

$$\left.\begin{aligned} &\mathbf{p}(\mathbf{q}_1,\mathbf{u}_1,t_1) - \bar{\mathbf{p}}_s = 0 \\ &\mathbf{u}_1 = \frac{1}{\Delta t}(\mathbf{q}_2 - \mathbf{q}_1) \end{aligned}\right\} \quad \Leftrightarrow \quad \left\{\begin{aligned} &\mathbf{u}_1 = \mathbf{u}_s \\ &\mathbf{q}_2 = \mathbf{q}_1 + \Delta t\, \mathbf{u}_s \end{aligned}\right. \tag{58}$$

2. k^{th} *step.* The coordinates $\mathbf{q}_{k-1}$ and $\mathbf{q}_k$ are known from the previous step. Solve (45) together with the contact laws (57) for $\mathbf{q}_{k+1}$, i.e. solve

$$\begin{aligned} &\mathbf{M}(\mathbf{q}_k,t_k)\big(\mathbf{u}_k - \mathbf{u}_{k-1}\big) - \mathbf{h}(\mathbf{q}_k,\mathbf{u}_{k-1},t_k)\Delta t = \mathbf{W}(\mathbf{q}_k,t_k)\mathbf{P}_k \\ &\mathbf{u}_k = \frac{1}{\Delta t}(\mathbf{q}_{k+1} - \mathbf{q}_k), \qquad \mathbf{u}_{k-1} = \frac{1}{\Delta t}(\mathbf{q}_k - \mathbf{q}_{k-1})\ , \\ &\text{where} \quad \forall i \in \mathcal{J} = \{i \,|\, g_i(\mathbf{q}_k) \le 0\}: \\ &- \xi_{Ni,k} \in \mathcal{N}_{\mathbb{R}_0^+}(P_{Ni,k}) \quad \text{with} \quad \xi_{Ni,k} \text{ as in (56)} \\ &- \boldsymbol{\xi}_{Ti,k} \in \mathcal{N}_{C_{Ti}(P_{Ni,k})}(\mathbf{P}_{Ti,k}) \quad \text{with} \quad \boldsymbol{\xi}_{Ti,k} \text{ as in (56)} \end{aligned} \tag{59}$$

3. Increase k by one and redo 2. if $t_k < t_f$.

4.2. Symmetric Moreau-type stepping scheme

1. *First step ($k=1$).* Set $\mathbf{q}_1 = \mathbf{q}_s$ and solve (50) together with the constitutive laws (57) for $\mathbf{q}_2$, i.e. solve

$$\begin{aligned} &\mathbf{p}(\mathbf{q}_1,\mathbf{u}_1,t_1) - \frac{1}{2}\Big(\mathbf{h}(\mathbf{q}_1,\mathbf{u}_1,t_1)\Delta t + \mathbf{W}(\mathbf{q}_1,t_1)\mathbf{P}_1\Big) - \bar{\mathbf{p}}_s = 0 \\ &\mathbf{u}_1 = \frac{1}{\Delta t}(\mathbf{q}_2 - \mathbf{q}_1), \qquad \mathbf{u}_0 = \mathbf{u}_s\ , \\ &\text{where} \quad \forall i \in \mathcal{J} = \{i \,|\, g_i(\mathbf{q}_1) \le 0\}: \\ &- \xi_{Ni,1} \in \mathcal{N}_{\mathbb{R}_0^+}(P_{Ni,1}) \quad \text{with} \quad \xi_{Ni,1} \text{ as in (56)} \\ &- \boldsymbol{\xi}_{Ti,1} \in \mathcal{N}_{C_{Ti}(P_{Ni,1})}(\mathbf{P}_{Ti,1}) \quad \text{with} \quad \boldsymbol{\xi}_{Ti,1} \text{ as in (56)} \end{aligned} \tag{60}$$

2. k^{th} *step.* The coordinates $\mathbf{q}_{k-1}$ and $\mathbf{q}_k$ are known from the previous step. Solve (49) together with the contact laws (57) for $\mathbf{q}_{k+1}$, i.e. solve

$$\begin{aligned} &\mathbf{M}(\mathbf{q}_k,t_k)\big(\mathbf{u}_k - \mathbf{u}_{k-1}\big) - \frac{1}{2}\Big(\mathbf{h}(\mathbf{q}_k,\mathbf{u}_{k-1},t_k) + \mathbf{h}(\mathbf{q}_k,\mathbf{u}_k,t_k)\Big)\Delta t = \mathbf{W}(\mathbf{q}_k,t_k)\mathbf{P}_k \\ &\mathbf{u}_k = \frac{1}{\Delta t}(\mathbf{q}_{k+1} - \mathbf{q}_k), \qquad \mathbf{u}_{k-1} = \frac{1}{\Delta t}(\mathbf{q}_k - \mathbf{q}_{k-1})\ , \\ &\text{where} \quad \forall i \in \mathcal{J} = \{i \,|\, g_i(\mathbf{q}_k) \le 0\}: \\ &- \xi_{Ni,k} \in \mathcal{N}_{\mathbb{R}_0^+}(P_{Ni,k}) \quad \text{with} \quad \xi_{Ni,k} \text{ as in (56)} \\ &- \boldsymbol{\xi}_{Ti,k} \in \mathcal{N}_{C_{Ti}(P_{Ni,k})}(\mathbf{P}_{Ti,k}) \quad \text{with} \quad \boldsymbol{\xi}_{Ti,k} \text{ as in (56)} \end{aligned} \tag{61}$$

3. Increase k by one and redo 2. if $t_k < t_f$.

DOI: 10.1002/nme

4.3. Variational Moreau-type stepping scheme [46]

1. *First step ($k = 1$).* Set $\mathbf{q}_1 = \mathbf{q}_s$ and solve (55) together with the constitutive laws (57) for $\mathbf{q}_2$, i.e. solve

$$\begin{aligned}
&\frac{1}{2}\Big(\mathbf{p}(\mathbf{q}_1,\mathbf{u}_1,t_1)+\mathbf{p}(\mathbf{q}_2,\mathbf{u}_1,t_2)-\mathbf{b}(\mathbf{q}_1,\mathbf{u}_1,t_1)\Delta t-\mathbf{W}(\mathbf{q}_1,t_1)\mathbf{P}_1\Big)-\bar{\mathbf{p}}_s=0\\
&\mathbf{u}_1=\frac{1}{\Delta t}(\mathbf{q}_2-\mathbf{q}_1),\qquad \mathbf{u}_0=\mathbf{u}_s\ ,\\
&\text{where}\quad \forall i\in\mathcal{J}=\{i\,|\,g_i(\mathbf{q}_1)\le 0\}:\\
&-\xi_{Ni,1}\in\mathcal{N}_{\mathbb{R}_0^+}(P_{Ni,1})\quad\text{with}\quad \xi_{Ni,1}\text{ as in (56)}\\
&-\boldsymbol{\xi}_{Ti,1}\in\mathcal{N}_{C_{Ti}(P_{Ni,1})}(\mathbf{P}_{Ti,1})\quad\text{with}\quad \boldsymbol{\xi}_{Ti,1}\text{ as in (56)}
\end{aligned}\tag{62}$$

2. *k^{th} step.* The coordinates $\mathbf{q}_{k-1}$ and $\mathbf{q}_k$ are known from the previous step. Solve (54) together with the contact laws (57) for $\mathbf{q}_{k+1}$, i.e. solve

$$\begin{aligned}
&\Big[\frac{1}{2}\Big(-\mathbf{p}(\mathbf{q}_k,\mathbf{u}_k,t_k)-\mathbf{p}(\mathbf{q}_{k+1},\mathbf{u}_k,t_{k+1})+\mathbf{p}(\mathbf{q}_{k-1},\mathbf{u}_{k-1},t_{k-1})+\mathbf{p}(\mathbf{q}_k,\mathbf{u}_{k-1},t_k)\Big)\\
&\quad+\frac{1}{2}\Big(\mathbf{b}(\mathbf{q}_k,\mathbf{u}_{k-1},t_k)+\mathbf{b}(\mathbf{q}_k,\mathbf{u}_k,t_k)\Big)\Delta t+\mathbf{W}(\mathbf{q}_k,t_k)\mathbf{P}_k\Big]=0\\
&\mathbf{u}_k=\frac{1}{\Delta t}(\mathbf{q}_{k+1}-\mathbf{q}_k),\qquad \mathbf{u}_{k-1}=\frac{1}{\Delta t}(\mathbf{q}_k-\mathbf{q}_{k-1})\ ,\\
&\text{where}\quad \forall i\in\mathcal{J}=\{i\,|\,g_i(\mathbf{q}_k)\le 0\}:\\
&-\xi_{Ni,k}\in\mathcal{N}_{\mathbb{R}_0^+}(P_{Ni,k})\quad\text{with}\quad \xi_{Ni,k}\text{ as in (56)}\\
&-\boldsymbol{\xi}_{Ti,k}\in\mathcal{N}_{C_{Ti}(P_{Ni,k})}(\mathbf{P}_{Ti,k})\quad\text{with}\quad \boldsymbol{\xi}_{Ti,k}\text{ as in (56)}
\end{aligned}\tag{63}$$

3. Increase k by one and redo 2. if $t_k < t_f$.

4.4. Remarks on the numerical schemes

For the solution of the normal cone inclusions arising due to the constitutive contact laws, the inclusion can be rewritten as an implicit proximal point equation. A discussion of different schemes of this type can be found in [10, 18, 45, 43]. For the special case of planar mechanical systems, the inclusions can be written in the form of a linear complementarity problem, as shown in [1, 47, 42]. The linear complementarity problem may be solved by Lemke's algorithm or some other schemes. We refer to [48] and [11] for details on linear complementarity problems and their numerical treatment. As a modification of Lemke's algorithm, a mechanically feasible pivoting strategy is proposed in [49]. Typically, Moreau's time-stepping scheme is assumed to have a possible impact, and therefore a velocity jump, at the midpoint of the considered integration step, see for example [2, 45, 42, 11]. The time instants t_k in the present formulation (59) are the possible impact times and correspond to the midpoints of the aforementioned common formulations.

5. NUMERICAL RESULTS

For autonomous mechanical systems described by a kinetic energy, which does only depend on the velocity $\dot{\mathbf{q}}$ of the system, and forces $\mathbf{f}$, which do not depend on the velocity, the three integrators coincide. This is for instance the case for the bouncing ball system as depicted in figure 1. This system consists of a mass m, which, under the influence of gravity with gravitational acceleration g, falls on a plane. The gap is equal to the position coordinate q. The bouncing ball system exhibits an accumulation of impacts. Namely, for a dissipative impact law, there is a sequence of infinitely

DOI: 10.1002/nme

many impacts in a finite time interval. The integrators derived in this paper can all overcome such an accumulation of impacts, as they do not resolve every single impact, cf. figure 2. This is due to the constant time step used in the schemes and due to the discrete contact laws (57), which take effect as soon as some contacts penetrate during the stepping process. This treatment of the contacts on velocity level represents a drawback of these contact laws, as discussed in the introduction. However, for many applications, the ability to overcome accumulations of impacts is considered more important than the price payed to achieve it, namely the contact penetration, which decreases with decreasing time steps. To prevent the contact penetration, [20, 21, 22] propose to introduce a Lagrange multiplier in the kinematic equations, which define the velocities in a first order formulation of the equations of motions. This multiplier allows to enforce the contact law on position level and can be seen as the adoption of the Gear-Gupta-Leimkuhler approach [50] to nonsmooth mechanical systems. Another approach to circumvent the contact penetration is proposed in [13, Appendix C], where in addition to velocity jumps also position jumps are allowed. The fact that the single impacts are not resolved, but all impacts happening during a time step are

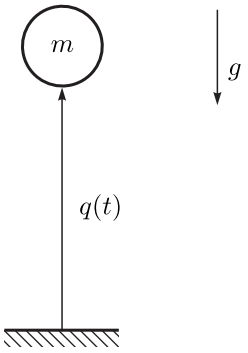

Figure 1. The bouncing ball system.

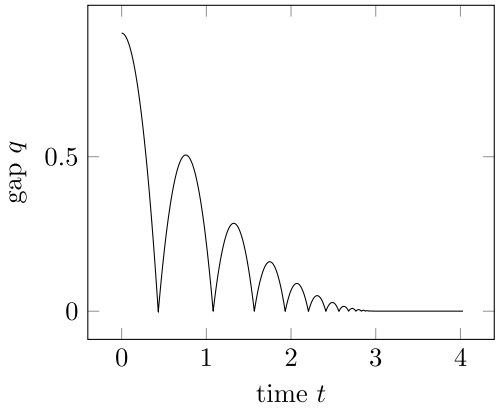

Figure 2. Gap of the bouncing ball calculated with Moreau's time-stepping scheme. Parameters: $m = 0.1$, $g = 9.81$, $e_N = 0.75$ and $\Delta t = 0.001$. Initial condition; $q(0) = 1$.

treated together by the discrete contact law, is of great importance for systems with many contacts. A very prominent example is the simulation of granular media, cf. for example [12, 13, 14, 15, 16]. It would be computationally very expensive to resolve all impacts for such systems. Moreover, such systems are likely to exhibit accumulations of impacts.

The spring pendulum depicted in figure 3 is an example system, which can be described by a nonconstant mass matrix. Therefore, the integrators derived in this paper do not coincide for the spring pendulum, which makes it suitable to compare the longterm energy behavior as well as the convergence of the schemes. The spring pendulum consists of a mass m, which is connected to one end of a linear spring with stiffness k. The other end of the spring is pivoted in point O. The actual length of the spring is denoted by $l(t)$ and its undeformed length is l_0. The deflection of the spring pendulum with respect to the vertical axis is $\varphi(t)$. The external forces acting on the system are the gravity, described by the gravitational constant g and contact forces arising from a frictionless contact with a vertical wall, where the contact is closed for $\varphi = 0$ and open for $\varphi > 0$. The contact between the wall and the pendulum is described by the restitution coefficient $e_N = 1$ modeling an elastic impact, which does not dissipate any energy. Therefore, the total energy $E = T + V$, with

$$T = \frac{1}{2}m(\dot{l}^2 + l^2\dot{\varphi}) \quad \text{and} \quad V = \frac{1}{2}k(l - l_0)^2 - mgl\cos\varphi\,, \tag{64}$$

is conserved along the motion, as the system is conservative also during time intervals between impacts. The energy error $e_E(t) = \frac{E(t)-E(0)}{E(0)}$ for motions of the spring pendulum, which are calculated with the three schemes derived above and the modified θ-method of Jean [3] for $\theta = 1/2$, are compared in figure 4. As the scheme presented in [3] is formulated for mechanical systems with

DOI: 10.1002/nme

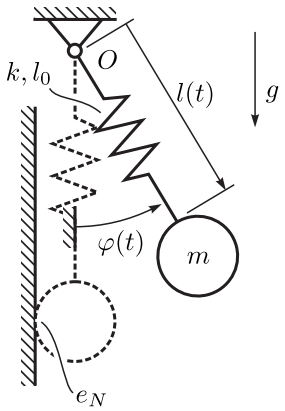

Figure 3. The spring pendulum.

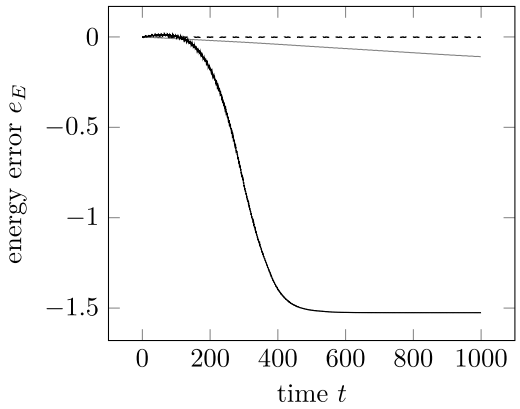

Figure 4. Energy error of the scheme of Moreau (solid), the symmetric Moreau-type scheme (dashed), the variational Moreau-type scheme (dashed) and the θ-method of Jean (gray) with $\theta = 1/2$. Parameters: $m = 1$, $l_0 = 1$, $k = 100$, $g = 9.81$, $e_N = 1$ and $\Delta t = 0.001$. Initial conditions: $\varphi(0) = \pi/4$, $l(0) = 1.1$, $\dot{\varphi}(0) = \dot{l}(0) = 0$.

constant mass matrix, we chose to evaluate the nonconstant mass matrix of the spring pendulum at the beginning of the time step, as suggested in [10]. In order to better understand figure 4, we note that the symmetric and variational Moreau-type stepping schemes are both symmetric schemes, meaning that inverting the scheme and changing the sign of the time step leads to the scheme itself. It is known for smooth time-reversible systems that errors of the conservation of first integrals are bounded if the numerical scheme is symmetric, cf. Hairer *et al.* [27, Sec. XI.3] for details and error bounds. As the spring pendulum is time-reversible between two subsequent impacts, the energy error is expected to be bounded between two impacts. Moreover, the variational Moreau-type stepping scheme is a variational integrator in the sense of discrete mechanics, as it is derived by discretizing the weak variational form of the virtual action. Such a discretization leads to a variational integrator, as shown in [26, Sec. 2.6.6], which are also known to perform well with respect to longterm energy conservation, cf. [27, Sec. IX.8] for details and error bounds. This represents an additional reason to explain the good conservation property of the variational Moreau-type stepping scheme between two impacts. Figure 4 confirms the good energy conservation properties of the two schemes and shows furthermore that no significant energy error occurs over the impact neither. In contrast to these two schemes, Moreau's stepping scheme dissipates a significant amount of energy. It can be observed, that the scheme dampens out the pendular motion of the system. This occurs approximately during the time interval $[0\ 500]$. After that, the motion of the spring pendulum is merely the motion of a vertically swinging harmonic oscillator, which has a constant mass matrix and for which the three integrators coincide. By what was said about the two other schemes, this explains the stabilization of the energy error for simulation times greater than 500. Also the modified θ-method dissipates energy, but overall, the energy error is smaller than the error of the time-stepping scheme of Moreau. For linear mechanical systems, the energy dissipation of the schemes of Moreau and Jean are studied in [51].

To study the convergence behavior for $\Delta t \to 0$ of the three schemes derived in this paper, the error

$$e_q(\Delta t) = \frac{1}{T}\int_0^T \left|\left|\mathbf{q}_{\mathrm{ref}}(t) - \mathbf{q}_{\mathrm{num}}(t;\Delta t)\right|\right|^2 \mathrm{d}t \tag{65}$$

is introduced, which measures the mean quadratic error between a reference motion $\mathbf{q}_{\mathrm{ref}}$ and the motion $\mathbf{q}_{\mathrm{num}}$ calculated by each of the schemes using the time step Δt. As reference solution for the convergence plot in figure 5, the motion computed with the symmetric Moreau-type stepping scheme with time step $\Delta t = 10^{-7}$ is used. Figure 5 shows that the stepping scheme of Moreau and the symmetric Moreau-type integrator are of the same order, but the error of the schemes

DOI: 10.1002/nme

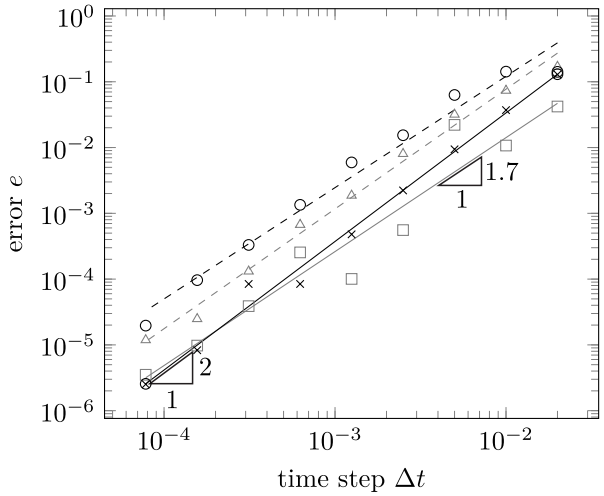

Figure 5. Convergence plot for the spring pendulum using the scheme of Moreau (black, dashed, ○), the symmetric Moreau-type scheme (gray, □), the variational Moreau-type scheme (black, ×) and the modified θ-method of Jean for $\theta = 1/2$ (gray, dashed, △).

approximately differs by one order of magnitude. Namely, for the same time step, the symmetric Moreau-type integrator has a ten times smaller error than the stepping scheme of Moreau. The convergence order of the variational Moreau-type scheme is slightly bigger than the order of the other schemes, but the error lies between the errors of the two other schemes. The convergence order of the modified θ-method lies between the convergence order of the symmetric and the variational Moreau-type scheme.

The woodpecker toy depicted in figure 6 was first introduced in [47]. It is a simple system containing multiple frictional contacts and is used as a benchmark for numerical integrators for systems with frictional contacts, cf. [10, 52]. The toy consists of a mechanism composed of a sleeve, a spring and a woodpecker. The mechanism can slide down a pole, as the sleeve is slightly larger than the diameter of the pole. Due to the frictional contacts between the pecker and the pole (contact point 1) as well as between the sleeve and the pole (contact points 2 and 3), the system has a limit cycle which corresponds to a kind of pitching motion. The rigid body model of the woodpecker toy is taken from [47]. As the mass matrix used in the model is constant and the non-contact forces do not depend on the velocity of the system, the three integrators derived in this paper coincide. The phase plot for the coordinate φ_M shown in figure 7 is computed by the three integrators and is in accordance with the phase plot shown in [53]. The woodpecker toy shows that all the three integrators are suitable for the simulation of a mechanical system with multiple frictional contacts.

6. CONCLUSIONS

With the principle of virtual action in its weak (with respect to time) variational form, we postulate a variational principle as the fundamental equation for the dynamics of finite dimensional mechanical systems containing frictional contact interactions. Since the principle of virtual action has to hold as an integral expression over a time interval, the forces, similar to the velocities, can be assumed to be special functions of locally bounded variations. This assumption allows to additively decompose the appearing contact forces into nonimpulsive contact forces, used to model persistent closed contacts and friction, and impulsive forces used to account for impacts. Besides the impulsive forces due to impacts, only the two impulsive forces on the boundary of the time interval are included. Using an integration by parts formula for SLBV-functions, the principle of virtual action is transformed into its strong variational form and induces directly the equality of measures or equivalently the equations of motion together with the impact equations – both systems of equations coming along

DOI: 10.1002/nme

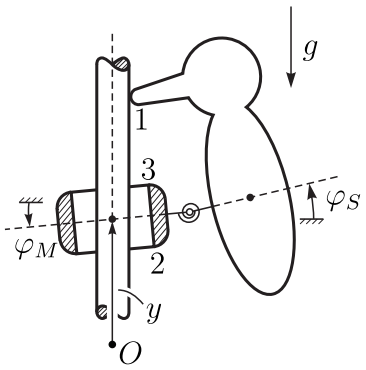

Figure 6. Woodpecker toy.

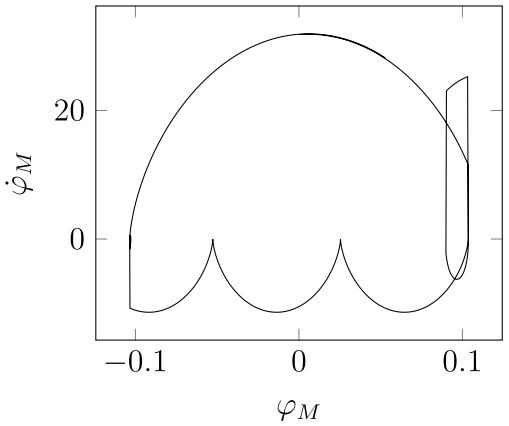

Figure 7. Phase plot for woodpecker toy computed with Moreau's time-stepping scheme, the symmetric and the variational Moreau-type stepping scheme.

with the same boundary conditions. Hence, the variational framework presented in this paper relates the equations of measures, which are often encountered in the description of nonsmooth mechanical systems, to analytical mechanics. To complete the description of the frictional contacts, the constitutive laws for the non-impulsive and impulsive contact forces, i.e. the contact and impact laws, are specified as normal cone inclusions.

A further merit of the paper is how this variational framework allows for a straightforward derivation of integration schemes for nonsmooth mechanical systems by discretizing the principle of virtual action with finite elements in time. The choice of some shape function in combination with some quadrature rule leads to various stepping schemes together with suitable initial conditions. In the discretized system, the constitutive laws for the impulsive and non-impulsive contact forces are treated on velocity-level as a unity by using a discrete contact law for the percussion increments in accordance with Moreau [2]. From this kind of the contact law the name Moreau-type integrators originates. In this paper, three integrators have been derived by using linear Lagrangian elements. Choosing a rectangle quadratrue rule in the strong variational form of the virtual action, the well-known Moreau time-stepping scheme follows. Deciding for a trapezoidal quadrature rule, the symmetric and the variational Moreau-type stepping scheme follow from the discretization of the strong and the weak variational form of the virtual action, respectively.

The comparison of the newly derived schemes to Moreau's time-stepping scheme and to the modified θ-method of Jean, shows the superiority of the new schemes in terms of energy conservation properties, accuracy and convergence. These good properties are achieved by choosing the trapezoidal rule which leads to symmetric schemes being known for their good numerical performance. Moreover, concerning the variational Moreau-type stepping scheme, the discretization of the weak variational form of the principle of virtual action leads to variational integrators in the sense of discrete mechanics. These variational integrators are known to preserve the structure of the underlying continuous time model, cf. [26]. Particularly, results from discrete mechanics on symplecticity and energy consistency of variational integrators directly apply to such a discretization.

To conclude, we have shown how the discretization of the principle of virtual action together with Moreau's treatment of contact forces combines the strengths of the discretization of measure differential inclusions with the advantages of the discretization of variational principles. We arrived in a well-structured way at new event-capturing integration schemes with excellent longterm simulation behavior.

DOI: 10.1002/nme

REFERENCES

[1] Ch. Glocker. *Set-Valued Force Laws: Dynamics of Non-Smooth Systems*, volume 1 of *Lecture Notes in Applied Mechanics*. Springer, 2001.

[2] J. J. Moreau. Unilateral contact and dry friction in finite freedom dynamics. In J. J. Moreau and P. D. Panagiotopoulos, editors, *Non-Smooth Mechanics and Applications. CISM Courses and Lectures*, pages 1–82. Springer, Wien, 1988.

[3] M. Jean. The non-smooth contact dynamics method. *Computer Methods in Applied Mechanics and Engineering*, 177(3-4):235–257, 1999.

[4] L. Paoli and M. Schatzman. A numerical scheme for impact problems I: The one-dimensional case. *SIAM Journal on Numerical Analysis*, 40(2):702–733, 2002.

[5] L. Paoli and M. Schatzman. A numerical scheme for impact problems II: The multidimensional case. *SIAM journal on numerical analysis*, 40(2):734–768, 2002.

[6] M. Anitescu, F. A. Potra, and D. E. Stewart. Time-stepping for three-dimensional rigid body dynamics. *Computer Methods in Applied Mechanics and Engineering*, 177:183–197, 1999.

[7] D. E. Stewart. A numerical method for friction problems with multiple contacts. *The Journal of the Australian Mathematical Society. Series B. Applied Mathematics*, 37:288–308, 1996.

[8] D. E. Stewart and J. C. Trinkle. An implicit time-stepping scheme for rigid body dynamics with inelastic collisions and Coulomb friction. *International Journal for Numerical Methods in Engineering*, 39:2673–2691, 1996.

[9] D. E. Stewart. Rigid-body dynamics with friction and impact. *SIAM Review*, 42(1):3–39, 2000.

[10] Ch. Studer. *Numerics of Unilateral Contacts and Friction: Modeling and Numerical Time Integration in Non-smooth Dynamics*, volume 47 of *Lecture Notes in Applied and Computational Mechanics*. Springer, Berlin, Heidelberg, 2009.

[11] V. Acary and B. Brogliato. *Numerical Methods for Nonsmooth Dynamical Systems: Applications in Mechanics and Electronics*, volume 35 of *Lecture Notes in Applied and Computational Mechanics*. Springer, Berlin, Heidelberg, 2008.

[12] J. J. Moreau. *Friction, Arching and Contact Dynamics*, chapter Numerical investigation of shear zones in granular materials, pages 233–247. World Scientific, 1997.

[13] G. E. Nützi. *Non-Smooth Granular Rigid Body Dynamics with Applications to Chute Flows*. PhD thesis, ETH Zurich, 2016.

[14] C. Nouguier-Lehon, B. Cambou, and E. Vincens. Influence of particle shape and angularity on the behaviour of granular materials: a numerical analysis. *International Journal for Numerical and Analytical Methods in Geomechanics*, 27:1207–1226, 2003.

[15] F. Radjai, D. E. Wolf, M. Jean, and J. J. Moreau. Bimodal character of stress transmission in granular packings. *Physical Review Letters*, 80(1):61–64, 1998.

[16] F. Radjai and S. Roux. Turbulentlike fluctuations in quasistatic flow of granular media. *Physical Review Letters*, 89(6):064302, 2002.

[17] O. Gonzalez. Time integration and discrete Hamiltonian systems. *Journal of Nonlinear Science*, 6(5):449–467, 1996.

[18] M. Möller. *Consistent Integrators for Non-Smooth Dynamical Systems*. PhD thesis, ETH Zurich, 2011.

DOI: 10.1002/nme

[19] V. Acary. Higher order event capturing time-stepping schemes for nonsmooth multibody systems with unilateral constraints and impacts. *Applied Numerical Mathematics*, 62:1259–1275, 2012.

[20] V. Acary. Projected event-capturing time-stepping schemes for nonsmooth mechanical systems with unilateral contact and Coulomb's friction. *Computer Methods in Applied Mechanics and Engineering*, 256:224–250, 2013.

[21] Q. Chen, V. Acary, G. Virlez, and O. Brüls. A nonsmooth generalized-α scheme for flexible multibody systems with unilateral constraints. *International Journal for Numerical Methods in Engineering*, 96(8):487–511, 2013.

[22] O. Brüls, V. Acary, and A. Cardona. Simultaneous enforcement of constraints at position and velocity levels in the nonsmooth generalized-α scheme. *Computer Methods in Applied Mechanics and Engineering*, 281:131–161, 2014.

[23] J. Har and K. Tamma. *Advances in Computational Dynamics of Particles, Materials and Structures*. Wiley, 2012.

[24] P. Betsch and P. Steinmann. Conservation properties of a time FE method. Part I: time-stepping schemes for N-body problems. *International Journal for Numerical Methods in Engineering*, 49(5):599–638, 2000.

[25] P. Betsch and P. Steinmann. Inherently energy conserving time finite elements for classical mechanics. *Journal of Computational Physics*, 160:88–116, 2000.

[26] J. E. Marsden and M. West. Discrete mechanics and variational integrators. *Acta Numerica 2001*, 10:357–514, 2001.

[27] E. Hairer, Ch. Lubich, and G. Wanner. *Geometric numerical integration: structure-preserving algorithms for ordinary differential equations*, volume 31 of *Springer Series in Computational Mathematics*. Springer Verlag, Berlin Heidelberg, second edition, 2006.

[28] R. C. Fetecau, J. E. Marsden, M. Ortiz, and M. West. Nonsmooth Lagrangian mechanics and variational collision integrators. *SIAM Journal on Applied Dynamical Systems*, 2(3):381–416, 2003.

[29] G. Johnson, S. Leyendecker, and M. Ortiz. Discontinuous variational time integrators for complex multibody collisions. *International Journal for Numerical Methods in Engineering*, 100(12):871–913, 2014.

[30] T. Schindler and V. Acary. Timestepping schemes for nonsmooth dynamics based on discontinuous Galerkin methods: definition and outlook. *Mathematics and Computers in Simulation*, 95:180–199, 2014.

[31] E. De Giorgi and L. Ambrosio. Un nuovo tipo di funzionale del calcolo delle variazioni. *Atti della Accademia Nazionale dei Lincei. Classe di Scienze Fisiche, Matematiche e Naturali. Rendiconti Lincei. Matematica e Applicazioni*, 82(2):199–210, 1988.

[32] G. Alberti and Mantegazza C. A note on the theory of sbv functions. *Bollettino Unione Matematica Italiana*, 11:375–382, 1997.

[33] E. Hellinger. Die Allgemeinen Ansätze der Mechanik der Kontinua. In *Encyklopädie der mathematischen Wissenschaften mit Einschluss ihrer Anwendungen*, volume IV-4, Heft 5. Springer, 1913.

[34] S. R. Eugster and F. dell'Isola. Exegesis of the introduction and sect. I from "Fundamentals of the mechanics of continua" by E. Hellinger. *Zeitschrift für angewandte Mathematik und Mechanik*, 97(4):477–506, 2017.

DOI: 10.1002/nme

[35] W. R. Hamilton. On a general method in dynamics; by which the study of the motions of all free systems of attracting or repelling points is reduced to the search and differentiation of one central relation, or characteristic function. *Philosophical transactions of the Royal Society of London*, 124:247–308, 1834.

[36] W. R. Hamilton. Second essay on a general method in dynamics. *Philosophical Transactions of the Royal Society of London*, 125:95–144, 1835.

[37] C. D. Bailey. Hamilton and the law of varying action revisited. *Foundations of Physics*, 34(9):1385–1406, 2004.

[38] L. Schwartz. *Théorie des distributions*. Hermann, Paris, 1966.

[39] Ch. Glocker. An introduction to impacts. In J. Haslinger and G. Stavroulakis, editors, *Nonsmooth Mechanics of Solids. CISM Courses and Lectures*, volume 485, pages 45–101. Springer, Wien, New York, 2006.

[40] B. Brogliato. *Nonsmooth Mechanics: Models, Dynamics and Control*. Communications and Control Engineering. Springer, third edition, 2016.

[41] J. G. Papastavridis. *Analytical Mechanics : A Comprehensive Treatise on the Dynamics of Constrained Systems (Reprint Edition)*. World Scientific Publishing Company, reprint edition, 2014.

[42] R. I. Leine and H. Nijmeijer. *Dynamics and Bifurcations of Non-Smooth Mechanical Systems*, volume 18 of *Lecture Notes in Applied and Computational Mechanics*. Springer, Berlin, Heidelberg, 2004.

[43] Ch. Glocker. Simulation of hard contacts with friction: an iterative projection method. In *Recent Trends in Dynamical Systems*, pages 493–515. Springer, 2013.

[44] J. Kujawski and C. S. Desai. Generalized time finite element algorithm for non-linear dynamic problems. *Engineering Computations*, 1(3):247–251, 1984.

[45] J. J. Moreau. Numerical aspects of the sweeping process. *Computer Methods in Applied Mechanics and Engineering*, 177:329 – 349, 1999.

[46] G. Capobianco and S. R. Eugster. A Moreau-type variational integrator. In *Proceedings im Applied Mathematics and Mechanics*, volume 16, pages 941–944. Wiley, 2016.

[47] Ch. Glocker. *Dynamik von Starrkörpersystemen mit Reibung und Stößen*. PhD thesis, TU München, 1995.

[48] K. G. Murty and F.-T. Yu. *Linear complementarity, linear and nonlinear programming*. Citeseer, 1988.

[49] K. Funk and F. Pfeiffer. A time-stepping algorithm for stiff mechanical systems with unilateral constraints. *Proceedings in Applied Mathematics and Mechanics*, 2:228–229, 2003.

[50] Ch. W. Gear, B. Leimkuhler, and G. K. Gupta. Automatic integration of Euler-Lagrange equations with constraints. *Journal of Computational and Applied Mathematics*, 12:77–90, 1985.

[51] V. Acary. Energy conservation and dissipation properties of time-integration methods for nonsmooth elastodynamics with contact. *ZAMM-Journal of Applied Mathematics and Mechanics/Zeitschrift für Angewandte Mathematik und Mechanik*, 2015.

[52] R. Zander, Th. Schindler, M. Friedrich, R. Huber, M. Förg, and H. Ulbrich. Non-smooth dynamics in academia and industry: recent work at tu münchen. *Acta Mechanica*, 195(1-4):167–183, 2008.

DOI: 10.1002/nme

[53] R. I. Leine, Ch. Glocker, and D. H. Van Campen. Nonlinear Dynamics of the Woodpecker Toy. *Proceedings of DETC 2001 ASME Symposium on Nonlinear Dynamics and Control In Engineering Systems*, September 9-12 2001. Pittsburgh, CD-ROM, DETC2001/VIB-21608.

DOI: 10.1002/nme