A dissipative discretization for large deformation frictionless dynamic contact problems

Jonathan William Youett, Oliver Sander

Abstract We present a discretization for dynamic large deformation contact problems without friction. Our model is based on Hamilton's principle, which avoids the explicit appearance of the contact forces. The resulting differential inclusion is discretized in time using a modified midpoint rule. This modification, which concerns the evaluation of the generalized gradient, allows to achieve energy dissipativity. For the space discretization we use a dual-basis mortar method. The resulting spatial algebraic problems are nonconvex minimization problems with nonconvex inequality constraints. These can be solved efficiently using a trust-region SQP framework with a monotone multigrid inner solver.

Keywords: frictionless dynamic contact, large deformations, modified midpoint rule, mortar method, multigrid SQP method

1 Introduction

In linear contact dynamics robust time discretizations have been developed on the basis of the Newmark method, cf. [8]. In nonlinear mechanics, however, most of these integrators lose their robustness as linear (spectral) stability is not sufficient anymore. It has been shown that energy dissipation is the main criterion for stability in nonlinear mechanics [2]. This motivates the construction of time discretization schemes that algorithmically enforce the conservation of energy and momentum.

In [5] Hartmann and Ramm combined the Generalized Energy–Momentum method [12] and a discrete contact velocity update [10] to construct a scheme con-

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serving energy and linear momentum. Hesch and Betsch used the discrete derivative proposed by Gonzales [4] which results in a momentum conserving method that conserves energy if a discrete persistency condition holds [6].

In all of the above models the contact forces appear explicitly, which requires the solution of generalized saddle point systems or the use of penalty methods. We avoid both issues by developing a variational integrator discretizing Hamilton's principle directly. This approach has been used by Kane et al. [7] in a model for contact problems between nonsmooth bodies. The approach leads to a differential inclusion involving generalized gradients [3], which has the advantage that no discretization of the contact forces is necessary, as they enter only implicitly. We propose a midpoint rule for the temporal discretization of the inclusion which is known to conserve momenta in the absence of contact [12]. To additionally achieve energy dissipation we further modify the resulting integrator by evaluating the generalized gradient at the new configuration instead of the averaged one. This is motivated by the proven dissipativity of a modified Newmark method for linearized contact problems, where the contact forces of the old time step are treated completely implicitly [8].

For the discretization of the contact constraints we apply a mortar method [13] with dual basis functions as proposed by Krause and Wohlmuth [14] for linear contact problems. The fully discrete problems that have to be solved in each time step are equivalent to nonconvex minimization problems which we solve using a trust-region SQP method with a monotone multigrid method as the interior solver [11].

2 The continuous problem

First we present the continuous problem, and briefly derive the weak equations of motion resulting from Hamilton's principle.

Nonlinear elasticity

Let $\Omega_1, \Omega_2 \subset \mathbb{R}^d$ be two domains denoting the reference configurations of two bodies. Their boundaries, with unit outer normals $\mathbf{n}^i$, are supposed to be decomposed into disjoint parts $\partial\Omega^i = \Gamma_D^i \cup \Gamma_N^i \cup \Gamma_C^i$. Let $\boldsymbol{\varphi}^i : \Omega_i \times [0,T] \to \mathbb{R}^d$, injective and sufficiently smooth, denote the current configuration of the body Ω_i.

In the framework of large deformations the equations of motion in reference coordinates are given in terms of the first Piola–Kirchhoff stress tensor $\mathbf{P}^i = \mathbf{P}^i(\boldsymbol{\varphi}^i)$, and read

$$\begin{aligned} \operatorname{div}(\mathbf{P}^i) + \mathbf{f}^i &= \rho\,\ddot{\boldsymbol{\varphi}}^i \quad \text{in } \Omega_i \\ \mathbf{P}^i\mathbf{n}^i &= \mathbf{t}^i \qquad \text{on } \Gamma_N^i \\ \boldsymbol{\varphi}^i &= \boldsymbol{\varphi}_D^i \quad \text{on } \Gamma_D^i, \end{aligned} \tag{1}$$

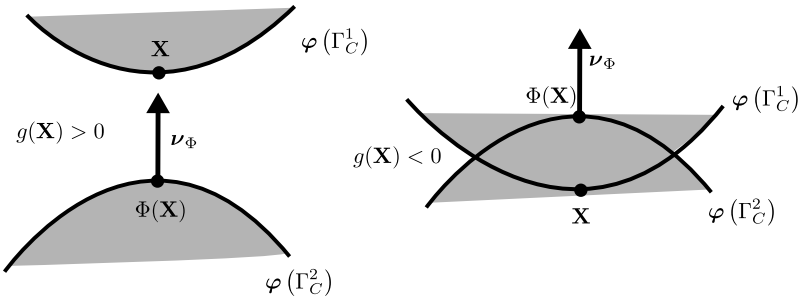


Fig. 1 Non-penetration condition. Left: Feasible configuration, $\boldsymbol{\nu_\Phi}$ points in the direction of $\mathbf{X} - \boldsymbol{\Phi}(\mathbf{X})$. Right: Unfeasible configuration, $\boldsymbol{\nu_\Phi}$ points away from $\mathbf{X} - \boldsymbol{\Phi}(\mathbf{X})$.

where $\mathbf{t}^i$ and $\boldsymbol{\varphi}_D^i$ are prescribed surface tractions and displacements, respectively, and ρ is the material density. The equations are supplemented with initial displacements and velocities

$$\boldsymbol{\varphi}^i(0) = \boldsymbol{\varphi}_0^i, \quad \dot{\boldsymbol{\varphi}}^i(0) = \mathbf{v}_0^i \quad \text{on } \Omega_i.$$

We consider hyperelastic materials only, i.e. materials for which there exists a strain energy functional W such that the first Piola–Kirchhoff stress is given by

$$\mathbf{P} = \frac{\partial W(\mathbf{X}, \mathbf{F})}{\partial \mathbf{F}},$$

where $\mathbf{F} = \nabla \boldsymbol{\varphi}$ denotes the deformation gradient.

Large deformation contact

We enforce non-penetration of the two bodies using the contact model introduced by Laursen [9]. The Γ_C^i, introduced above, denote the parts of the boundaries that may come into contact. We identify these two surfaces with each other by the time-dependent closest point projection

$$\begin{aligned} \boldsymbol{\Phi} \;:\; \Gamma_C^1 \times [0,T] &\longrightarrow \Gamma_C^2 \\ \boldsymbol{\Phi}(\mathbf{X},t) &:= \underset{\mathbf{Y} \in \Gamma_C^2}{\arg\min} \left\| \boldsymbol{\varphi}^1(\mathbf{X},t) - \boldsymbol{\varphi}^2(\mathbf{Y},t) \right\|. \end{aligned}$$

This projection defines a vector field on the deformed contact patch $\boldsymbol{\varphi}^2(\Gamma_C^2)$ by

$$\boldsymbol{\nu}_{\boldsymbol{\Phi}}(\mathbf{X},t) := \frac{\boldsymbol{\varphi}^1(\mathbf{X},t) - \boldsymbol{\varphi}^2 \circ \boldsymbol{\Phi}(\mathbf{X},t)}{||\boldsymbol{\varphi}^1(\mathbf{X},t) - \boldsymbol{\varphi}^2 \circ \boldsymbol{\Phi}(\mathbf{X},t)||} \operatorname{sgn}(\boldsymbol{\varphi}),$$

where $\operatorname{sgn}(\boldsymbol{\varphi})$ is chosen such that $\boldsymbol{\nu}_\Phi(t)$ points outward of $\boldsymbol{\varphi}^2(\Gamma_C^2)$. Note that $\boldsymbol{\nu}_\Phi$ is normal to $\boldsymbol{\varphi}^2(\Gamma_C^2)$ since Φ is a best approximation. The gap function $g : \Gamma_C^1 \times [0,T] \to \mathbb{R}$ can then be defined as

$$g(\mathbf{X},t) := \boldsymbol{\nu}_\Phi(\mathbf{X},t) \cdot \big(\boldsymbol{\varphi}^1(\mathbf{X},t) - \boldsymbol{\varphi}^2 \circ \Phi(\mathbf{X},t)\big),$$

and non-penetration is achieved by enforcing

$$g(\mathbf{X},t) \geq 0 \quad \forall (\mathbf{X},t) \in \Gamma_C^1 \times [0,T]. \tag{2}$$

To see why this works note that for unfeasible deformations the vectors $\boldsymbol{\varphi}^1 - \boldsymbol{\varphi}^2 \circ \Phi$ and $\boldsymbol{\nu}_\Phi$ point in opposite directions by the choice of $\operatorname{sgn}(\boldsymbol{\varphi})$, and the gap function becomes negative (Fig. 1).

Weak equations of motion

In contact dynamics it is common to add the virtual work of the unknown contact forces directly to the weak equations of motions, which results in a variational equation for the deformations and the contact tractions [5, 6]. We use a different approach and derive weak equations of motion by applying Hamilton's principle to a nonsmooth Lagrangian [7]. This results in a differential inclusion which has the advantage that the contact forces do not enter explicitly and thus will not have to be discretized. For simplicity we assume vanishing external forces $\mathbf{f}^i = 0$, $\mathbf{t}^i = 0$. Also for simplicity we assume that the Dirichlet boundary values, if present at all, are constant in time. We write $\mathbf{H}_D^1(\Omega)$ for the standard first-order Sobolev space of d-valued functions that satisfy the Dirichlet condition.

Hamilton's principle states that the evolution of a dynamical system during a time interval $[0,T]$ with Lagrangian $L(\mathbf{u},\dot{\mathbf{u}})$ is a stationary point of the action integral

$$\mathscr{I}(\boldsymbol{\varphi}) := \int_0^T L(\boldsymbol{\varphi},\dot{\boldsymbol{\varphi}})\,dt.$$

For hyperelastic materials the Lagrangian is of the form

$$L(\boldsymbol{\varphi},\dot{\boldsymbol{\varphi}}) = \rho(\dot{\boldsymbol{\varphi}},\dot{\boldsymbol{\varphi}})_{\mathbf{L}^2(\Omega)} - \int_\Omega W(\nabla\boldsymbol{\varphi})\,dx,$$

and the corresponding Euler–Lagrange equations are (1).

We incorporate non-penetration of the two bodies by adding the indicator function $I_{\mathscr{K}}$ of the nonconvex set of feasible solutions

$$\mathscr{K} := \big\{\mathbf{v} \in H_D^1(\Omega) \;:\; g(\mathbf{X}) \geq 0 \text{ a.e. on } \Gamma_C^1\big\}$$

to the potential energy, which ensures that the trajectory stays feasible at all times. The resulting new Lagrangian

$$\tilde{L}(\boldsymbol{\varphi}, \dot{\boldsymbol{\varphi}}) := L(\boldsymbol{\varphi}, \dot{\boldsymbol{\varphi}}) - I_{\mathscr{K}}(\boldsymbol{\varphi}). \tag{3}$$

is nonsmooth and, due to the nonconvexity of $\mathscr{K}$, not even subdifferentiable. Nevertheless it is possible to derive Euler–Lagrange equations by using the concept of generalized gradients $\boldsymbol{\partial}$ in the sense of Rockafellar and Clarke [3], for which the following first-order optimality criterion has been shown:

Proposition 1 ([3], Prop. 2.4.11). *Let X be a Banach space and $f : X \to [-\infty, +\infty]$ be finite at $\mathbf{u}$. If $\mathbf{u}$ is a local extremal point of f then $0 \in \boldsymbol{\partial} f(\mathbf{u})$.*

Application of this stationary condition to the nonsmooth Lagrangian (3) leads to the Euler–Lagrange differential inclusion

$$0 \in \boldsymbol{\partial}\tilde{L} = \rho\ddot{\boldsymbol{\varphi}} + \mathbf{F}^{\text{int}}(\boldsymbol{\varphi}) + \boldsymbol{\partial} I_{\mathscr{K}}(\boldsymbol{\varphi}), \tag{4}$$

where the internal forces $\mathbf{F}^{\text{int}}$ are given by

$$\mathbf{F}^{\text{int}}(\boldsymbol{\varphi})\mathbf{v} := \int_{\Omega} \mathbf{P}(\boldsymbol{\varphi}) : \nabla \mathbf{v}\, dx.$$

3 Discretization

For the discretization of the problem we use the method of time layers, i.e. discretize first in time and then in space. We will start with the description of the modified midpoint rule and then state the finite element and mortar discretization of the contact constraints.

3.1 Time discretization

Let $0 = t^0 < t^1 < \ldots < t^N = T$ be a subdivision of the time interval $[0, T]$ into—for simplicity—equidistant time steps $\tau = t^{k+1} - t^k$, and denote by $\boldsymbol{\varphi}^n = \boldsymbol{\varphi}(t^n)$ the numerical approximation of $\boldsymbol{\varphi}$ at time step t^n. For the time discretization of the differential inclusion (4) we construct a modified midpoint rule by approximating the velocity and displacement by second order Taylor expansion

$$\begin{aligned}
\boldsymbol{\varphi}^{n+1} &= \boldsymbol{\varphi}^n + \tau\dot{\boldsymbol{\varphi}}^n + \frac{\tau^2}{4}(\ddot{\boldsymbol{\varphi}}^{n+1} + \ddot{\boldsymbol{\varphi}}^n), \\
\dot{\boldsymbol{\varphi}}^{n+1} &= \dot{\boldsymbol{\varphi}}^n + \frac{\tau}{2}(\ddot{\boldsymbol{\varphi}}^{n+1} + \ddot{\boldsymbol{\varphi}}^n),
\end{aligned}$$

and evaluating the differential inclusion at the averaged midpoints

$$\boldsymbol{\varphi}^{n+1/2} := \frac{\boldsymbol{\varphi}^{n+1} + \boldsymbol{\varphi}^n}{2}.$$

This leads to the following differential inclusion and update formula

$$0 \in \frac{2}{\tau^2}\rho(\boldsymbol{\varphi}^{n+1} - \boldsymbol{\varphi}^n - \tau\dot{\boldsymbol{\varphi}}^n) + \mathbf{F}^{\text{int}}(\boldsymbol{\varphi}^{n+1/2}) + \partial I_{\mathscr{K}}(\boldsymbol{\varphi}^{n+1/2}),$$
$$\dot{\boldsymbol{\varphi}}^{n+1} = \frac{2}{\tau}(\boldsymbol{\varphi}^{n+1} - \boldsymbol{\varphi}^n) - \dot{\boldsymbol{\varphi}}^n.$$

In the absence of contact this midpoint rule is known not to be energy dissipative in general [12]. As energy dissipation is the main criteria for stability we propose the following modification which is motivated by a similar construction by Kane et al. [7] for the Newmark method, where the contact forces of the old time step are treated implicitly. We evaluate the generalized gradient $\partial I_{\mathscr{K}}$ at the new displacement $\boldsymbol{\varphi}^{n+1}$ instead of the averaged midpoint. The modified time discrete inclusion then reads

$$0 \in \frac{2}{\tau^2}\rho(\boldsymbol{\varphi}^{n+1} - \boldsymbol{\varphi}^n - \tau\dot{\boldsymbol{\varphi}}^n) + \mathbf{F}^{\text{int}}(\boldsymbol{\varphi}^{n+1/2}) + \partial I_{\mathscr{K}}(\boldsymbol{\varphi}^{n+1}).$$

While there is no proof of the dissipativity of this time integrator, we nevertheless observe in the numerical experiments in Section 4 a much better energy behaviour. In particular, the total energy of the system stays bounded.

3.2 Spatial discretization

Assume that Ω_1 and Ω_2 are discretized by conforming grids $\Omega_{1,h}$ and $\Omega_{2,h}$. We discretize the nonlinear elasticity problem in the space $\mathbf{S}_h$ of first-order Lagrangian finite elements, and the non-penetration constraint using a mortar method [13]. This means that we replace the strong non-penetration constraint (2) by a weak integral one on the deformed contact surface $\boldsymbol{\varphi}_h(\Gamma_C^1)$

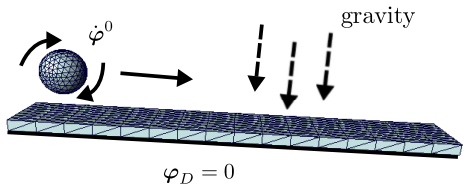
$$\int_{\boldsymbol{\varphi}_h(\Gamma_C^1)} g\,\theta_h\,ds \geq 0 \quad \forall\,\theta_h \in M_h^+.$$

As the mortar space M_h^+ we choose the positive cone of the dual basis mortar space [13], which is characterized by a biorthogonality relation with the nodal basis functions of $\boldsymbol{S}_h$. The corresponding set of admissible solutions is

$$\mathscr{K}_h = \left\{\mathbf{v}_h \in S_h(\Omega_h) : \int_{\boldsymbol{\varphi}_h(\Gamma_C^1)} g\,\theta_h\,ds \geq 0 \quad \forall\,\theta_h \in M_h^+\right\}.$$

Note that $\mathscr{K}_h$ is again closed and nonconvex, but that it is not a subset of $\mathscr{K}$. The fully discrete problem reads

Fig. 2 Initial configuration



$$0 \in \frac{2}{\tau^2}\rho(\boldsymbol{\varphi}_h^{n+1} - \boldsymbol{\varphi}_h^n - \tau\dot{\boldsymbol{\varphi}}_h^n) + \mathbf{F}^{\text{int}}(\boldsymbol{\varphi}_h^{n+1/2}) + \partial I_{\mathscr{K}_h}(\boldsymbol{\varphi}_h^{n+1}), \tag{5}$$

$$\dot{\boldsymbol{\varphi}}_h^{n+1} = \frac{2}{\tau}(\boldsymbol{\varphi}_h^{n+1} - \boldsymbol{\varphi}_h^n) - \dot{\boldsymbol{\varphi}}_h^n.$$

By Proposition 1 we get the following characterization of the discrete problem

Lemma 1. *A solution* $\boldsymbol{\varphi}_h^{n+1}$ *of the differential inclusion* (5) *is a stationary point of the functional*

$$\mathscr{J}(\mathbf{v}) := \frac{1}{\tau^2}\int_{\Omega_h}(\rho\mathbf{v}, \mathbf{v} - 2\boldsymbol{\varphi}_h^n - 2\tau\dot{\boldsymbol{\varphi}}_h^n)\,dx + 2\int_{\Omega_h} W\left(\frac{\mathbf{v}+\boldsymbol{\varphi}_h^n}{2}\right)dx$$

in the discrete admissible set $\mathscr{K}_h$.

We expect the stationary point to be a minimizer when the time step size is small. This suggests to treat (5) as a minimization problem for a nonconvex but smooth energy functional, with nonconvex inequality constraints.

4 Numerical results

We will now examine the energy behaviour of the proposed scheme for a St. Venant–Kirchhoff material with Young's modulus $E = 1\,\text{MPa}$ and Poisson ratio $\nu = 0.3$ and density $\rho = 0.1\,\text{g/cm}^3$. As the reference configuration we consider a rectangular body that is fixed by prescribing homogeneous Dirichlet values on the lower boundary. A spherical body is located at a distance of 2 mm above and is given an initial angular velocity of $(0,2,0)$ m/s plus a translational velocity of $(2,0,0)$ m/s. Additionally both bodies are subjected to gravity. As the result, the ball bounces along the foundation (Figure 2).

The discrete spatial problems are solved by a Trust-Region SQP method, cf. [11] for more details. For the inner quadratic problems with linearized constraints we use a monotone multigrid method [14], which allows to solve even large problems efficiently. The implementation is based on the DUNE libraries [1].

The left of Figure 3 shows the total energy for different time step sizes. There is no increase in energy, and for small enough time step sizes there is some energy loss only when the ball hits the foundation. The loss of energy reduces with smaller

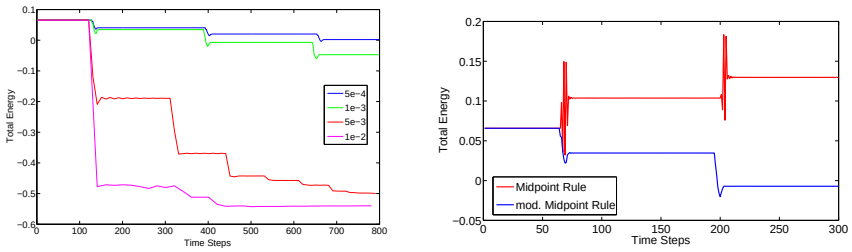


Fig. 3 Total Energy. Left: Energy over time for different time step sizes. Right: Comparison of the proposed integrator with the unmodified midpoint rule.

time step sizes. At each impact we also see small oscillations that are typical for symplectic integrators.

Next we compare the proposed method against the unmodified midpoint rule for the same model problem with a fixed time step size of $\tau = 0.001\,\mathrm{s}$. In the right of Figure 3 the total energy of both methods is shown, and one can observe the improved behaviour of the modified midpoint rule. While the unmodified midpoint rule gains energy at each impact, the modified rule stays practically dissipative.

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