

Mixed interpretation and extensions of the equivalent mass matrix approach for elastodynamics with contact

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Abstract

The present paper highlights the idea that the mass redistribution technique introduced by Khenous, Laborde and Renard [17,18] for elastodynamics with impact, can be reinterpreted as a mixed formulation in displacements and velocities in which a special compatibility condition is enforced. Such a formulation opens the route to various extensions and to variational integrators for impact problems, potentially with variational time adaption. Those ideas are exemplified in the design of such integrators and various mass redistribution schemes.

Key words: Contact, Mixed formulations, Equivalent Mass Matrix, Variational integration

1 Introduction

Let u denote the displacement field over a body $\Omega \subset \mathbb{R}^3$ undergoing small deformations. The standard analysis of the linearized elastodynamics equations on the time interval $[0, T]$ provides that (see [37])

$$u \in C^0(0, T; H^1(\Omega)) \cap C^1(0, T; L^2(\Omega)).$$

Consequently, at any time $t \in [0, T]$ the displacements $u(t)$ and velocities $\dot{u}(t)$ do not have *a priori* the same regularity. Nevertheless, most of the time integration schemes proposed in the framework of elastodynamics define the discrete

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velocity \dot{u}_n at time $t_n = n\Delta t$ on the same discretization space as displacements. The drawbacks could be of great concern for non-smooth problems, as space oscillations are likely to occur.

In the present paper, we propose the use of separate spaces for displacements and velocities. The relation between both is enforced under weak form against a Lagrange multiplier space; such functions represent linear momenta. After elimination, the corresponding constraint simply results into the modification of the mass operator. Various time integration schemes can then be written in the present framework, including energy/momenta conserving schemes [39,29,11,15] or variational schemes [32]. We show in particular that no consistency error is introduced by the approach and that optimal convergence by time step refinement is retained in the linearized framework provided proper spaces are chosen.

The approach results into natural mass lumping, often used to obtain diagonal approximations. Diagonal approximations of mass matrices have been mainly developed in view of the efficiency of explicit time integration schemes [10] but may be also useful to some implicit schemes [23,24]. But more importantly, mass lumping has been shown helpful to eliminate numerical dispersion in wave propagation problems [40,22]. Various methods have been used over the past to generate such matrices, from "row-summing" [34] to Newton-Cotes quadrature points, aiming at maximizing accuracy even to the point of accurately accounting for rotations (cf. [9] and the references therein). The interest of the present approach is to provide a natural variational framework with guaranteed stability and convergence.

Well beyond the issue of regularity for velocities and displacements, the approach allows for the definition of specific models in which only part of the displacements are involved in the effective velocities.

We also illustrate the interest of the present setting to formulate variational schemes in a very flexible way. Since the early works of Maeda, Veselov, Suris and Mac Kay, variational schemes have been the object of numerous publications by Marsden *et al.* (cf. [32] for a review as well as [25,30]). They constitute a route to symplectic time integration (see [13]) through the discretization of the Lagrange function of the problem. Moreover, it has been showed that such an approach can be conciliated with an energy preserving vision of time integration. The key is the definition of the time step as an independent variable enabling to solve the additional conservation constraint (cf. [32]), though the question of existence remains open. An additional step has been made in [31] through the use of the Hamilton-Pontryagin principle; it allows for an independent definition of the energies and the displacements-velocities relationship. The present work advocates in addition, the choice of independent spaces in agreement with the geometric formulation of the method.

The ultimate goal of the paper lies in the application of this mixed approach to contact dynamics. Contact dynamics has always been confronted to specific difficulties concerning its discretization in space and time. Mortar approximations (cf [5,6,3,19,35]) have been proven to be superior in terms of optimal convergence in space. They have been extended to use bi-orthogonal Lagrange multipliers enabling elimination of the constraint [43,20,21] or discontinuous Lagrange multipliers enabling local support of the constrained basis [4,16]. Moreover, efforts have been made in the field of geometry smoothing [36]. Regarding time discretization, energy-preserving integrators have been extensively developed around the notion of persistency condition [27,1,28,15]. The extreme sensitivity of the problem has been highlighted by Moreau [33] who has shown that solutions are not uniquely defined and exhibit poor regularity in the absence of a persistency condition. In spite of these contributions, the numerical solution of dynamical contact problems may exhibit oscillations in space and time [17,18,12] directly linked to the adopted discretization. All these symptoms may very well be related to the lack of mathematical foundations [8] for variational inequalities involving dynamic terms. In specific cases nevertheless, existence of solutions can be established, but with extremely poor regularity [2].

Recently, Khenous, Laborde and Renard have shown [17,18,38] that in the space discrete framework, removing all mass from the displacement degrees of freedom orthogonal to the contact surface brings regularity back into the problem. The resulting problem exhibits Lipschitz regularity in time and achieves energy conservation due to the automatic satisfaction of the persistency condition; additionally, standard time discretization strategies lead to discrete evolutions showing surprisingly good energy evolution properties. The underlying idea behind mass lumping is to split the problem between an unconstrained elastodynamic problem and a static boundary problem handling the non-penetration constraint. The mass redistribution, either performed by the initial optimization procedure of the authors or by the use of special Gauss points on boundary macro-elements [12], preserves both the barycenter and the inertia tensor of the structure. Considering that for industrial structures the geometry is never represented exactly anyway, simpler strategies can be used [41]. In order to preserve the possibility to transfer linear momentum – and therefore to trigger tangential waves – on the contact interface, the mass action should only be modified along the normal direction. The semi-discrete solutions have also been proved to converge in the visco-elastic case by space refinement, as shown by [7].

Our present contribution consists in showing that mass redistribution does not constitute a variational crime in regards to the Lagrange principle underlying constrained elastodynamics. We establish herein that the idea is equivalent to choosing a couple of velocity and displacement spaces satisfying a strong persistency condition on the contact boundary of the domain. As we show,

optimal convergence follows for the fully discrete problem in time, at least with prescribed contact forces.

The present paper is organized as follows. Section 2.1 introduces the variational principle underlying the proposed mixed approach, while Section 2.2 shows energy/momenta conserving discretizations can be easily formulated. In Section 2.3, we analyze a simple first-order scheme and show that optimal convergence by time-step refinement is retained for the mixed approach; more complex schemes could be handled in the exact same way. Section 2.4 exploits the present framework for variational schemes.

Section 3 is devoted to the re-interpretation of Khenous- Laborde- Renard's mass lumping technique as a mixed method, in which velocity and displacement spaces satisfy a strong persistency condition. Some numerical examples are presented in Section 4; they illustrate the benefits of the present approach in terms of regularity in time of the pressure field and its good behavior by time-step refinement.

2 Mixed framework in velocities-displacements

2.1 Formal setting

To allow for independent space discretizations of displacements and velocities in the framework of nonlinear elastodynamics, let us turn back to the following action,

$$S(\varphi, p, \lambda) = \frac{1}{2} \int_0^T \int_{\Omega} \varrho |p|^2 - \int_0^T \int_{\Omega} W(\nabla \varphi) - \int_0^T \int_{\Omega} \lambda \cdot (p - \partial_t \varphi),$$

defined for every $(\varphi, p, \lambda) \in L^\infty(0, T; \Phi) \cap H^1(0, T; L^2(\Omega)^3) \times L^2(0, T; \mathcal{P}_{\varphi(t)}) \times L^2(0, T; \Lambda_{\varphi(t)})$. The velocity-displacement relationship is enforced under weak form. The hyper-elastic stored energy function in terms of the deformation gradient is denoted by $W(F)$ and the material density by $\varrho > 0$. The deformation manifold is denoted as Φ . For every $\varphi \in \Phi$, the velocity space is the vector space \mathcal{P}_φ and the space of Lagrange multipliers is the vector space Λ_φ . According to the Lagrange principle, the deformation states are known at the beginning and the end of the trajectories, i.e. $\varphi(0, \cdot) = \varphi_0$ and $\varphi(T, \cdot) = \varphi_T$. Rendering the action stationary with respect to the field of deformation φ reads

$$\int_0^T \int_{\Omega} \lambda \cdot \partial_t \delta \varphi - \int_0^T \int_{\Omega} \partial_F W(\nabla \varphi) : \nabla \delta \varphi = 0 \quad \forall \delta \varphi. \quad (1)$$

The action stationarity with respect to $p \in L^2(0, T; \mathcal{P}_{\varphi(t)})$ provides, for almost every time $t \in [0, T]$,

$$\int_{\Omega} \lambda(t) \cdot \delta p = \int_{\Omega} \varrho p(t) \cdot \delta p \quad \forall \delta p \in \mathcal{P}_{\varphi(t)}, \quad (2)$$

which we denote by $\lambda(t) = \mathbb{P}_{\Lambda_{\varphi(t)}}(\varrho p(t))$. The action stationarity with respect to $\lambda \in L^2(0, T; \Lambda_{\varphi(t)})$ implies, for almost every time $t \in [0, T]$,

$$\int_{\Omega} p(t) \cdot \delta \lambda = \int_{\Omega} \partial_t \varphi(t) \cdot \delta \lambda \quad \forall \delta \lambda \in \Lambda_{\varphi(t)}, \quad (3)$$

which we denote by $p(t) = \mathbb{P}_{\mathcal{P}_{\varphi(t)}}(\partial_t \varphi(t))$.

Owing to relations (2) and (3), equation (1) reads

$$- \int_0^T \int_{\Omega} \varrho \mathbb{P}_{\mathcal{P}}(\partial_t \varphi) \cdot \mathbb{P}_{\mathcal{P}}(\partial_t \delta \varphi) + \int_0^T \int_{\Omega} \partial_F W(\nabla \varphi) : \nabla \delta \varphi = 0, \quad (4)$$

for every $\delta \varphi$. For clarity purpose, we have omitted the dependence of the projectors with respect to the deformation state $\varphi(t)$. Observe the velocity space manifests itself through the reduction of the mass operator on the left hand side. Assuming sufficient regularity in time, it follows that

$$\int_{\Omega} \varrho \partial_t \mathbb{P}_{\mathcal{P}}(\partial_t \varphi) \cdot \mathbb{P}_{\mathcal{P}}(\delta \varphi) + \int_{\Omega} \partial_F W(\nabla \varphi) : \nabla \delta \varphi = 0 \quad \forall \delta \varphi \in T_{\varphi(t)} \Phi, \quad (5)$$

where $T_{\varphi(t)} \Phi$ stands for the tangent space to the deformation manifold at deformation $\varphi(t)$.

We have assumed that $\mathbb{P}_{\mathcal{P}}(\partial_t \square) = \partial_t \mathbb{P}_{\mathcal{P}} \square$; it is the case for continuous projectors $\mathbb{P}_{\mathcal{P}}$ whenever $\partial_t \square \in \mathcal{P}$.

2.2 Energy-momenta conserving strategies

We now proceed to define a time integration scheme exploiting the aforementioned mixed structure and look for $(\varphi_n, p_n, \lambda_n)_{1 \leq n \leq N}$ satisfying

$$\begin{cases} \int_{\Omega} \frac{1}{\Delta t} (\lambda_{n+1} - \lambda_n) \cdot \delta \varphi + \int_{\Omega} \Pi_{n+1/2} : \nabla \delta \varphi = 0 & \forall \delta \varphi \in T_{\varphi} \Phi, \\ \int_{\Omega} \frac{1}{2} (p_n + p_{n+1}) \cdot \delta \lambda = \int_{\Omega} \frac{1}{\Delta t} (\varphi_{n+1} - \varphi_n) \cdot \delta \lambda & \forall \delta \lambda \in T_{\lambda} \Lambda, \\ \int_{\Omega} \lambda_n \cdot \delta p = \int_{\Omega} \varrho p_n \cdot \delta p & \forall \delta p \in T_p \mathcal{P}. \end{cases} \quad (6)$$

We assume as in [39,29,11,15] that the algorithmic first Piola-Kirchhoff stress tensor $\Pi_{n+1/2}$ which approximates $\partial_F W(\nabla\varphi_{n+1/2})$ satisfies

$$\Pi_{n+1/2} = \frac{1}{2}\nabla(\varphi_n + \varphi_{n+1}) \cdot \Sigma_{n+1/2}, \quad (7)$$

where $\Sigma_{n+1/2}$ is symmetric and

$$\frac{1}{2}\Sigma_{n+1/2} : (C_{n+1} - C_n) = W(\nabla\varphi_{n+1}) - W(\nabla\varphi_n). \quad (8)$$

$C_n = (\nabla\varphi_n)^\top \cdot (\nabla\varphi_n)$ is the right Cauchy-Green strain tensor.

Remark 1 *This idea has been developed through the seminal work of Simo and Tarnow [39] ; $\Sigma_{n+1/2}$ can be computed using the approach of Laursen and Meng [29] or can be written explicitly using the finite difference correction proposed by Gonzalez [11], with various extensions to incompressibility, visco-elasticity and contact formulation from Hauret and Le Tallec [15].*

Theorem 1 *Under assumptions (7), (8), the time integration scheme (6) achieves exact conservation of the discrete energy*

$$\mathcal{E}_n = \frac{1}{2} \int_{\Omega} \varrho |p_n|^2 + \int_{\Omega} W(\nabla\varphi_n),$$

and of the discrete linear momentum $\mathcal{I}_n = \int_{\Omega} \lambda_n$ provided translations are allowed in the space of admissible displacements. Assuming that rotations are allowed and that for every $p \in \mathcal{P}$, $\lambda \in \Lambda$ and $a \in \mathbb{R}^3$, one has $a \times p \in \mathcal{P}$ and $a \times \lambda \in \Lambda$, the discrete angular momentum $\mathcal{J}_n = \int_{\Omega} \varphi_n \times \lambda_n$ also gets preserved.

Proof. Energy conservation is obtained by using the test function $\delta\varphi = \frac{1}{\Delta t}(\varphi_{n+1} - \varphi_n)$ in the system (6). Using (6).2 and (6).3, the inertial term leads to

$$\begin{aligned} \int_{\Omega} \frac{\lambda_{n+1} - \lambda_n}{\Delta t} \cdot \frac{\varphi_{n+1} - \varphi_n}{\Delta t} &= \int_{\Omega} \frac{\lambda_{n+1} - \lambda_n}{\Delta t} \cdot \frac{p_n + p_{n+1}}{2} \\ &= \int_{\Omega} \varrho \frac{p_{n+1} - p_n}{\Delta t} \cdot \frac{p_n + p_{n+1}}{2} \\ &= \frac{1}{\Delta t} \left(\frac{1}{2} \int_{\Omega} \varrho |p_{n+1}|^2 - \frac{1}{2} \int_{\Omega} \varrho |p_n|^2 \right), \end{aligned} \quad (9)$$

which corresponds to the increase of kinetic energy between successive time steps. Owing to assumptions (7) and (8), the hyperelastic contribution reads

$$\begin{aligned}
& \frac{1}{\Delta t} \int_{\Omega} \Pi_{n+1/2} : \nabla(\varphi_{n+1} - \varphi_n) \\
&= \frac{1}{2\Delta t} \int_{\Omega} \Sigma_{n+1/2} : (C_{n+1} - C_n) = \frac{1}{\Delta t} \int_{\Omega} (W(\nabla\varphi_{n+1}) - W(\nabla\varphi_n)),
\end{aligned}$$

which proves the announced energy conservation after summation with (9).

Linear momentum conservation is straightforward using constant displacement fields $\delta\varphi$ in (6). Concerning angular momentum, we use $\delta\varphi = \frac{1}{2}a \times (\varphi_n + \varphi_{n+1})$, and the elastic contribution vanishes since

$$\frac{1}{2} \int_{\Omega} \Pi_{n+1/2} : [a \times \nabla(\varphi_n + \varphi_{n+1})] = \int_{\Omega} [F_{n+1/2} \cdot \Sigma_{n+1/2} \cdot F_{n+1/2}^{\top}] : \mathbb{J}_a = 0,$$

where we have used assumption (7). We have introduced $F_{n+1/2} = \frac{1}{2}\nabla(\varphi_n + \varphi_{n+1})$ and \mathbb{J}_a denotes the (skew-symmetric) matrix such that $\mathbb{J}_a x = a \times x$ for every $x \in \mathbb{R}^3$; the above conclusion follows by observing the symmetry of $[F_{n+1/2} \cdot \Sigma_{n+1/2} \cdot F_{n+1/2}^{\top}]$. The inertial term reads

$$\int_{\Omega} \frac{\lambda_{n+1} - \lambda_n}{\Delta t} \cdot \left[a \times \frac{\varphi_n + \varphi_{n+1}}{2} \right] = a \cdot \int_{\Omega} \frac{\varphi_n + \varphi_{n+1}}{2} \times \frac{\lambda_{n+1} - \lambda_n}{\Delta t}, \quad (10)$$

and one observes from the second and third equations in (6) that

$$\begin{aligned}
& \int_{\Omega} \frac{\varphi_{n+1} - \varphi_n}{\Delta t} \times \frac{\lambda_n + \lambda_{n+1}}{2} = \int_{\Omega} \frac{p_n + p_{n+1}}{2} \times \frac{\lambda_n + \lambda_{n+1}}{2} \\
&= \int_{\Omega} \varrho \frac{p_n + p_{n+1}}{2} \times \frac{p_n + p_{n+1}}{2} = 0,
\end{aligned}$$

which summed to (10) entails the announced conservation of the angular momentum.

Observe the present scheme can be implemented as

$$\begin{cases} \int_{\Omega} \varrho \mathbb{P}_{\mathcal{P}} \frac{\dot{\varphi}_{n+1} - \dot{\varphi}_n}{\Delta t} \cdot \mathbb{P}_{\mathcal{P}} \delta\varphi + \int_{\Omega} \Pi_{n+1/2} : \nabla \delta\varphi = 0 & \forall \delta\varphi \in T_{\varphi} \Phi, \\ \frac{1}{2}(\dot{\varphi}_n + \dot{\varphi}_{n+1}) = \frac{1}{\Delta t}(\varphi_{n+1} - \varphi_n), \end{cases} \quad (11)$$

with the introduction of the velocity field $(\dot{\varphi}_n) \in \Phi$. In this setting, we get

$$p_n = \mathbb{P}_{\mathcal{P}} \dot{\varphi}_n.$$

It is worth noticing that the displacement-velocity relationship is enforced pointwisely in space, as usual. The present scheme corresponds to the simple implementation of a standard conservative scheme in presence of a modified mass operator.

2.3 Optimal convergence

Let us consider the elastodynamic problem consisting of finding

$$u \in C^0(0, T; H_*^1(\Omega)) \cap C^1(0, T; L^2(\Omega))$$

with

$$H_*^1(\Omega) = \{v \in H^1(\Omega)^3, \quad v|_{\Gamma_D} = 0\}$$

such that for every $t \in [0, T]$

$$\partial_t m(\dot{u}(t), v) + a(u(t), v) = \ell(v), \quad \forall v \in H_*^1(\Omega), \quad (12)$$

where the time derivative ∂_t is in the sense of distributions, ℓ is a continuous linear form on $H_*^1(\Omega)$, and

$$m(v, w) = \int_{\Omega} \varrho v \cdot w \quad \forall v, w \in L^2(\Omega),$$

$$a(v, w) = \int_{\Omega} (\mathbf{E} : \varepsilon(v)) : \varepsilon(w) \quad \forall v, w \in H_*^1(\Omega).$$

Above, \mathbf{E} is the fourth order elasticity tensor, and $\varepsilon(v)$ the symmetric part of the gradient of v .

Introducing the discrete times $t_n = n \Delta t$, the discrete vector spaces $\mathcal{P}_h \subset L^2(\Omega)$, $\Lambda_h \subset L^2(\Omega)$, $\Phi_h \subset H_*^1(\Omega)$ for velocities, impulses and displacements respectively as in the previous section, we consider the first order scheme defining the discrete solution by

$$\begin{cases} m \left(\mathbb{P}_{\mathcal{P}_h} \frac{\dot{u}_{n+1}^h - \dot{u}_n^h}{\Delta t}, \mathbb{P}_{\mathcal{P}_h} v^h \right) + a(u_{n+1}^h, v^h) = \ell(v^h) & \forall v^h \in \Phi_h, \\ \dot{u}_{n+1}^h = \frac{u_{n+1}^h - u_n^h}{\Delta t}. \end{cases} \quad (13)$$

Remark 2 *We could have analyzed the second order variant coming from the linearization of the scheme proposed in the previous section, in which:*

$$\frac{\dot{u}_n^h + \dot{u}_{n+1}^h}{2} = \frac{u_{n+1}^h - u_n^h}{\Delta t}.$$

The extension is rather straightforward (cf. [14, Proposition 4.10; Chapter 4; p 154]) considering the key-aspects of the proof, as mentioned in Remark 3.

We assume

Assumption 1 (Approximation Error) *There exists a positive constant $C > 0$ independent of h , such that for every $u \in H^2(\Omega)^3$,*

$$\inf_{u_h \in \Phi_h} \|u - u_h\|_{H^1(\Omega)^3} \leq C h |u|_{H^2(\Omega)^3}$$

and for every $p \in H^1(\Omega)^3$,

$$\inf_{p_h \in \mathcal{P}_h} \|p - p_h\|_{L^2(\Omega)^3} \leq C h |p|_{H^1(\Omega)^3}.$$

Assumption 2 (Projection stability) *There exists a positive constant $C > 0$ independent of h , such that for every $\lambda_h \in \Lambda_h$,*

$$\sup_{p_h \in \mathcal{P}_h \setminus \{0\}} \frac{\int_{\Omega} p_h \cdot \lambda_h}{\|p_h\|_{L^2(\Omega)^3}} \geq \beta \|\lambda_h\|_{L^2(\Omega)^3}.$$

This assumption classically implies the existence of a projection $\mathbb{P}_{\mathcal{P}_h}$, and the following stability inequality with a positive constant C such that

$$\|\mathbb{P}_{\mathcal{P}_h} v\|_{L^2(\Omega)^3} \leq C \|v\|_{L^2(\Omega)^3}, \quad (14)$$

for every $v \in L^2(\Omega)^3$.

The error committed in the mixed framework depicted above can be estimated in the setting provided by the energetic method from [42]. For analysis purpose, we denote

$$\mathbf{e}u_n = \mathbb{P}_{\Phi_h} u(t_n) - u_n^h \quad \mathbf{e}v_n = v_n - \dot{u}_n^h$$

where

$$a(\mathbb{P}_{\Phi_h} v, w) = a(v, w) \quad \forall w \in \Phi_h,$$

and

$$v_{n+1} = \mathbb{P}_{\Phi_h} \frac{u(t_{n+1}) - u(t_n)}{\Delta t}.$$

Theorem 2 (Convergence) *Assumptions 1 and 2 are supposed to be satisfied. Let $u \in C^0(0, T; H^2(\Omega)^3) \cap C^1(0, T; H^1(\Omega)^3) \cap C^2(0, T; H^1(\Omega)^3) \cap C^3(0, T; L^2(\Omega)^3)$ be the solution of (12) and $(u_n^h, \dot{u}_n^h)_n$ be the discrete solution of (13). There exists a constant $C > 0$ independent of h , of the time step Δt , of the domain size, and the material parameters ϱ , \mathbf{E} , such that*

$$\begin{aligned}
& \|\dot{u}(t_n) - \dot{u}_n^h\|_m + \|u(t_n) - u_n^h\|_a \leq \\
\leq & C \left(\|\mathbb{P}_{\Phi_h} \dot{u}(t_0) - \dot{u}_0^h\|_m + \|\mathbb{P}_{\Phi_h} u(t_0) - u_0^h\|_a \right. \\
& + \|\varrho\|_{L^\infty(\Omega)}^{1/2} \left(h t_{n+1} \|\ddot{u}\|_{L^\infty(0,T;H^1(\Omega)^3)} + \Delta t t_{n+1} \|\ddot{u}\|_{L^\infty(0,T;L^2(\Omega)^3)}^2 \right) \\
& + \frac{\|\varrho\|_{L^\infty(\Omega)}}{\theta} \left(h t_{n+1} \|\ddot{u}\|_{L^\infty(0,T;L^2(\Omega)^3)} + h \|\ddot{u}\|_{L^\infty(0,T;L^2(\Omega)^3)} \right) \\
& + \|\varrho\|_{L^\infty(\Omega)}^{1/2} \left(\Delta t \|\ddot{u}\|_{L^\infty(0,T;L^2(\Omega)^3)} + h \|\dot{u}\|_{L^\infty(0,T;H^1(\Omega)^3)} \right) \\
& \left. + \|\mathbf{E}\|_{L^\infty(\Omega)^{3 \times 3}}^{1/2} h \|u\|_{L^\infty(0,T;H^2(\Omega)^3)} \right).
\end{aligned}$$

We have introduced the norms $\|\square\|_m = m(\square, \square)^{1/2}$ and $\|\square\|_a = a(\square, \square)^{1/2}$; the coercivity constant θ is such that

$$a(v, v) \geq \theta \left(\frac{1}{\text{diam}(\Omega)^2} \int_{\Omega} |v|^2 + \int_{\Omega} |\nabla v|^2 \right) \quad \forall v \in H_*^1(\Omega).$$

Proof. Substracting (13) to (12) at time $t = t_{n+1}$, one gets for every $v \in \Phi_h$,

$$\begin{aligned}
& m \left(\mathbb{P}_{\mathcal{P}_h} \frac{\mathbf{e}v_{n+1} - \mathbf{e}v_n}{\Delta t}, \mathbb{P}_{\mathcal{P}_h} v \right) + a(\mathbf{e}u_{n+1}, v) \\
= & m \left(\mathbb{P}_{\mathcal{P}_h} \frac{v_{n+1} - v_n}{\Delta t} - \ddot{u}(t_{n+1}), \mathbb{P}_{\mathcal{P}_h} v \right) + m(\ddot{u}(t_{n+1}), \mathbb{P}_{\mathcal{P}_h} v - v). \quad (15)
\end{aligned}$$

Using $v = (\mathbf{e}u_{n+1} - \mathbf{e}u_n)/\Delta t$ in (15) and owing to the fact that

$$\frac{\mathbf{e}u_{n+1} - \mathbf{e}u_n}{\Delta t} = \mathbf{e}v_{n+1},$$

it follows after summation over n , multiplication by Δt and using the Cauchy-Schwarz inequality that

$$\begin{aligned}
& \frac{1}{2} m(\mathbb{P}_{\mathcal{P}_h} \mathbf{e}v_{n+1}, \mathbb{P}_{\mathcal{P}_h} \mathbf{e}v_{n+1}) + \frac{1}{2} a(\mathbf{e}u_{n+1}, \mathbf{e}u_{n+1}) \\
\leq & \frac{1}{2} m(\mathbb{P}_{\mathcal{P}_h} \mathbf{e}v_0, \mathbb{P}_{\mathcal{P}_h} \mathbf{e}v_0) + \frac{1}{2} a(\mathbf{e}u_0, \mathbf{e}u_0) + \sum_{k=0}^n I_k + III. \quad (16)
\end{aligned}$$

Introducing

$$III = \left(\sum_{k=0}^n \int_{\Omega} \varrho |\mathbb{P}_{\mathcal{P}_h} \mathbf{e}v_{k+1}|^2 \right)^{1/2},$$

the following approximation errors are involved,

$$\begin{aligned}
& \sum_{k=0}^n I_k = \Delta t \sum_{k=0}^n m \left(\mathbb{P}_{\mathcal{P}_h} \frac{\mathbf{v}_{k+1} - \mathbf{v}_k}{\Delta t} - \ddot{u}(t_{k+1}), \mathbb{P}_{\mathcal{P}_h} \mathbf{e}\mathbf{v}_{k+1} \right) \\
& \leq \frac{\Delta t}{\tau} (III) \left(\tau^2 \sum_{k=0}^n \int_{\Omega} \varrho \left| \mathbb{P}_{\mathcal{P}_h} \mathbb{P}_{\Phi_h} \frac{u(t_{k+1}) - 2u(t_k) + u(t_{k-1}))}{\Delta t^2} - \ddot{u}(t_{k+1}) \right|^2 \right)^{1/2} \\
& \leq \frac{\Delta t}{\tau} \left[2 \tau^2 \sum_{k=0}^n \int_{\Omega} \varrho |\mathbb{P}_{\mathcal{P}_h} (\mathbb{P}_{\Phi_h} a_k - \ddot{u}(t_{k+1}))|^2 \right. \\
& \quad \left. + 2 \tau^2 \sum_{k=0}^n \int_{\Omega} \varrho |\mathbb{P}_{\mathcal{P}_h} \ddot{u}(t_{k+1}) - \ddot{u}(t_{k+1})|^2 \right]^{1/2} \times (III) \\
& \leq C \frac{\Delta t}{\tau} \left[\tau^2 \|\varrho\|_{L^\infty(\Omega)} \sum_{k=0}^n \|\mathbb{P}_{\Phi_h} a_k - a_k\|_{L^2(\Omega)^3}^2 \right. \\
& \quad \left. + \tau^2 \|\varrho\|_{L^\infty(\Omega)} \sum_{k=0}^n \|a_k - \ddot{u}(t_{k+1})\|_{L^2(\Omega)^3}^2 \right. \\
& \quad \left. + \tau^2 \|\varrho\|_{L^\infty(\Omega)} \sum_{k=0}^n \|\mathbb{P}_{\mathcal{P}_h} \ddot{u}(t_{k+1}) - \ddot{u}(t_{k+1})\|_{L^2(\Omega)^3}^2 \right]^{1/2} \times (III) \\
& \leq C \frac{T}{2\tau} \left[h^2 \tau^2 \|\varrho\|_{L^\infty(\Omega)} \|\ddot{u}\|_{L^\infty(0,T;H^1(\Omega)^3)}^2 + \Delta t^2 \tau^2 \|\varrho\|_{L^\infty(\Omega)} \|\ddot{u}\|_{L^\infty(0,T;L^2(\Omega)^3)}^2 \right. \\
& \quad \left. + h^2 \tau^2 \|\varrho\|_{L^\infty(\Omega)} \|\ddot{u}\|_{L^\infty(0,T;H^1(\Omega)^3)}^2 \right] + \frac{\Delta t}{2\tau} \left(\sum_{k=0}^n \int_{\Omega} \varrho |\mathbb{P}_{\mathcal{P}_h} \mathbf{e}\mathbf{v}_{k+1}|^2 \right), \quad (17)
\end{aligned}$$

for every τ . We have exploited the definition of $(\mathbf{v}_k)_{k=0,\dots,n+1}$, have introduced $u(t_{-1}) = u(t_0) - \dot{u}(t_0) \Delta t$ in view of employing uniform notation, and $a_k = \frac{u(t_{k+1}) - 2u(t_k) + u(t_{k-1}))}{\Delta t^2}$ to shorten the expressions. We have used the triangular inequality, the stability inequality (14) and the approximation properties from Assumption 1. Similarly, denoting $\mathbb{Q} = \mathbb{P}_{\mathcal{P}_h} - Id$ we get:

$$\begin{aligned}
& \sum_{k=0}^n II_k = \Delta t \sum_{k=0}^n m (\ddot{u}(t_{k+1}), \mathbb{P}_{\mathcal{P}_h} \mathbf{e}\mathbf{v}_{k+1} - \mathbf{e}\mathbf{v}_{k+1}) \\
& = \Delta t \sum_{k=0}^n m (\ddot{u}(t_{k+1}), \mathbb{Q}\mathbf{e}\mathbf{v}_{k+1}) = \sum_{k=0}^n m (\ddot{u}(t_{k+1}), \mathbb{Q}(\mathbf{e}\mathbf{u}_{k+1} - \mathbf{e}\mathbf{u}_k)) \\
& = \sum_{k=1}^n m (\ddot{u}(t_k) - \ddot{u}(t_{k+1}), \mathbb{Q}\mathbf{e}\mathbf{u}_k) + m (\ddot{u}(t_{n+1}), \mathbb{Q}\mathbf{e}\mathbf{u}_{n+1}) - m (\ddot{u}(t_1), \mathbb{Q}\mathbf{e}\mathbf{u}_0) \\
& \leq C \frac{T}{\tau\theta} \left(h^2 \tau^2 \|\varrho\|_{L^\infty(\Omega)}^2 \|\ddot{u}\|_{L^\infty(0,T;L^2(\Omega)^3)}^2 \right) + \theta \frac{\Delta t}{2\tau} \sum_{k=1}^n |\mathbf{e}\mathbf{u}_k|_{H^1(\Omega)^3}^2 \\
& \quad + C \frac{h^2}{\theta} \|\varrho\|_{L^\infty(\Omega)}^2 \|\ddot{u}\|_{L^\infty(0,T;L^2(\Omega)^3)}^2 + \frac{\theta}{4} \left(|\mathbf{e}\mathbf{u}_{n+1}|_{H^1(\Omega)^3}^2 + |\mathbf{e}\mathbf{u}_0|_{H^1(\Omega)^3}^2 \right),
\end{aligned}$$

hence choosing θ as the coercivity constant of the bilinear form a , we get:

$$\begin{aligned}
\sum_{k=0}^n II_k &\leq C \frac{T}{\tau \theta} \left(h^2 \tau^2 \|\varrho\|_{L^\infty(\Omega)}^2 \|\ddot{u}\|_{L^\infty(0,T;L^2(\Omega)^3)}^2 \right) \\
&+ C \frac{1}{\theta} h^2 \|\varrho\|_{L^\infty(\Omega)}^2 \|\ddot{u}\|_{L^\infty(0,T;L^2(\Omega)^3)}^2 \\
&+ \frac{\Delta t}{2\tau} \sum_{k=1}^n a(\mathbf{e}u_k, \mathbf{e}u_k) + \frac{1}{4} (a(\mathbf{e}u_{n+1}, \mathbf{e}u_{n+1}) + a(\mathbf{e}u_0, \mathbf{e}u_0)).
\end{aligned}$$

Equations (16), (17) and (18) provide

$$\begin{aligned}
&\frac{1}{2} \left(1 - \frac{\Delta t}{\tau} \right) m(\mathbb{P}_{\mathcal{P}_h} \mathbf{e}v_{n+1}, \mathbb{P}_{\mathcal{P}_h} \mathbf{e}v_{n+1}) + \frac{1}{4} a(\mathbf{e}u_{n+1}, \mathbf{e}u_{n+1}) \\
&\leq \frac{1}{2} m(\mathbb{P}_{\mathcal{P}_h} \mathbf{e}v_0, \mathbb{P}_{\mathcal{P}_h} \mathbf{e}v_0) + \frac{3}{4} a(\mathbf{e}u_0, \mathbf{e}u_0) \\
&+ C \|\rho\|_{L^\infty(\Omega)^3} \frac{T}{\tau} \left(h^2 \tau^2 \|\ddot{u}\|_{L^\infty(0,T;H^1(\Omega)^3)}^2 + \Delta t^2 \tau^2 \|\ddot{u}\|_{L^\infty(0,T;L^2(\Omega)^3)}^2 \right) \\
&+ C \|\rho\|_{L^\infty(\Omega)^3}^2 \frac{1}{\theta} \left(h^2 \tau^2 \|\ddot{u}\|_{L^\infty(0,T;L^2(\Omega)^3)}^2 + h^2 \|\ddot{u}\|_{L^\infty(0,T;L^2(\Omega)^3)}^2 \right) \\
&+ \frac{\Delta t}{\tau} \sum_{k=1}^n \left(\frac{1}{2} m(\mathbb{P}_{\mathcal{P}_h} \mathbf{e}v_k, \mathbb{P}_{\mathcal{P}_h} \mathbf{e}v_k) + \frac{1}{2} a(\mathbf{e}u_{k+1}, \mathbf{e}u_{k+1}) \right).
\end{aligned}$$

Consequently, assuming $\Delta t \leq \frac{\tau}{2}$ to get the bound $\left(1 - \frac{\Delta t}{\tau}\right) \geq \frac{1}{2}$ on the left hand side, the discrete Gronwall's lemma (see for instance [14, lemma 4.13, p. 175]) establishes that

$$\begin{aligned}
&m(\mathbb{P}_{\mathcal{P}_h} \mathbf{e}v_{n+1}, \mathbb{P}_{\mathcal{P}_h} \mathbf{e}v_{n+1}) + a(\mathbf{e}u_{n+1}, \mathbf{e}u_{n+1}) \\
&\leq C \frac{T}{\tau} \left(1 + \frac{2\Delta t}{\tau} \right)^{n+1} \left(m(\mathbb{P}_{\mathcal{P}_h} \mathbf{e}v_0, \mathbb{P}_{\mathcal{P}_h} \mathbf{e}v_0) + a(\mathbf{e}u_0, \mathbf{e}u_0) \right. \\
&+ \|\varrho\|_{L^\infty(\Omega)} \left(h^2 \tau^2 \|\ddot{u}\|_{L^\infty(0,T;H^1(\Omega)^3)}^2 + \Delta t^2 \tau^2 \|\ddot{u}\|_{L^\infty(0,T;L^2(\Omega)^3)}^2 \right) \\
&\left. + \frac{\|\varrho\|_{L^\infty(\Omega)}^2}{\theta} \left(h^2 \tau^2 \|\ddot{u}\|_{L^\infty(0,T;L^2(\Omega)^3)}^2 + h^2 \|\ddot{u}\|_{L^\infty(0,T;L^2(\Omega)^3)}^2 \right) \right). \tag{18}
\end{aligned}$$

We choose $T = \tau = t_{n+1}$, from which

$$\left(1 + \frac{2\Delta t}{t_{n+1}} \right)^{n+1} = \exp \left(\frac{t_{n+1}}{\Delta t} \log \left(1 + \frac{2\Delta t}{t_{n+1}} \right) \right)$$

remains bounded by e^2 . The announced result follows from the triangular inequalities

$$\begin{aligned}
&\|u(t_{n+1}) - u_{n+1}^h\|_a \leq \|u(t_{n+1}) - \mathbb{P}_{\Phi_h} u(t_{n+1})\|_a + \|\mathbf{e}u_{n+1}\|_a \\
&\leq C \|\mathbf{E}\|_{L^\infty(\Omega)^{3 \times 3}}^{1/2} h |u|_{L^\infty(0,T;H^2(\Omega)^3)} + \|\mathbf{e}u_{n+1}\|_a,
\end{aligned}$$

where $\|\square\|_a = a(\square, \square)^{1/2}$ and introducing $\mathbf{v}_{n+1} = (u(t_{n+1}) - u(t_n))/\Delta t$,

$$\begin{aligned} \|\dot{u}(t_{n+1}) - \dot{u}_{n+1}^h\|_m &\leq \|\dot{u}(t_{n+1}) - \mathbf{v}_{n+1}\|_m + \|\mathbf{v}_{n+1} - \mathbb{P}_{\Phi_h} \mathbf{v}_{n+1}\|_m + \|\mathbf{e}\mathbf{v}_{n+1}\|_m \\ &\leq \|\varrho\|_{L^\infty(\Omega)}^{1/2} \left(\Delta t \|\ddot{u}\|_{L^\infty(0,T;L^2(\Omega)^3)} + Ch \|\dot{u}\|_{L^\infty(0,T;H^1(\Omega)^3)} \right) + \|\mathbf{e}\mathbf{v}_{n+1}\|_m, \end{aligned}$$

with $\|\square\|_m = m(\square, \square)^{1/2}$.

Remark 3 *The key-differences introduced by mass-lumping concern the approximation of velocities in \mathcal{P}_h (estimation of $\sum I_k$) and the discrete time integration by parts required to estimate $\sum II_k$; it implies a h -convergence controlled by $\|\ddot{u}\|_{L^\infty(0,T;L^2(\Omega)^3)}$.*

Remark 4 *We have assumed that Γ_D has a positive measure, and therefore the static equilibrium is well-posed. If not, the proof can be adapted by decomposing the displacements between rigid body motions and the $m(\cdot, \cdot)$ -orthogonal displacements. The same result easily follows.*

Remark 5 *Since no consistency error is involved in the previous analysis, it appears the mixed approach does not introduce any variational crime. An alternative proof is given by B. Wohlmuth and C. Hager in [12].*

Remark 6 *In presence of a visco-elastic term, additional compactness is obtained on velocities and the numerical solution can be proven to converge weakly to the solution of the continuous problem in space and time, as recently proven in [7]. The existence of the continuous visco-elastic solution being known, the convergence could also be handled from the analysis in [44]. The interesting result is that the regularization implied by the mass modification disappears at the continuous limit.*

2.4 Application to variational integrators

The mixed approach can also be employed to design variational integrators. In this framework, the mixed term will not only be used to define the displacements-velocities relationship from the point of view of the space approximation, but also from the point of view of time discretization schemes.

Variational schemes make use of a time discrete version of the Lagrange principle. The main interest is the straightforward obtention of symplectic schemes for which a discrete version of the Noether's theorem holds (see [32]). As a consequence, discrete linear and angular momenta are automatically preserved. Moreover, when the time step is small enough, good energy conservation is

achieved. The case of stiff systems remain a source of debate though, since fine time steps may be required to benefit from such a promise.

Remark 7 *Assuming the system has a Lipschitz constant L , good energy properties and accuracy of the trajectories can be proven for $\Delta t L \leq cte$ as proven in [13, Theorem 7.6, p. 365], even though the authors show numerically that this condition may be too pessimistic.*

Nevertheless, observe that symplectic time integration might be designed to conserve energy as well, provided adapted time steps are specifically computed.

2.4.1 Mixed Lagrange principle with time reparametrization

We turn here to the more general case of the action

$$\mathcal{S}(q) = \int_0^T L(q(t), \dot{q}(t), t) dt,$$

acting on $q : [0, T] \rightarrow Q$ with prescribed values $q(0)$ and $q(T)$. To allow for conciliation of symplecticity and energy conservation in the discrete framework, Marsden and West [32] propose to consider a separate description of the time line $\tau : [0, S] \rightarrow [0, T]$ and the state $\xi : [0, S] \rightarrow Q$. Introducing $q(t) = \xi \circ \tau^{-1}(t)$, a modified action with time reparametrization can now be considered

$$\mathcal{S}(\xi, \tau) = \int_0^S L\left(\xi(s), c(s)^{-1} \frac{d\xi}{ds}(s), \tau(s)\right) c(s) ds,$$

where $c(s) = \frac{d\tau}{ds}(s)$. Introducing in addition a weak linear relationship between velocities and states, we propose the mixed action:

$$\mathfrak{S}(\xi, \tau, p, \lambda) = \int_0^S L(\xi(s), p(s), \tau(s)) c(s) ds - \int_0^S \left\langle \lambda(s), p(s) - c(s)^{-1} \frac{d\xi}{ds}(s) \right\rangle c(s) ds.$$

From now on, we assume smoothness of the solution in time. Stationarity with respect to p reads

$$\frac{\partial L}{\partial \dot{q}} \cdot \delta p - \langle \lambda, \delta p \rangle = 0 \quad \forall \delta p \in T_p \mathcal{P},$$

which we denote by

$$\lambda = \mathbb{P}_\Lambda \left(\frac{\partial L}{\partial \dot{q}} \right).$$

Stationarity with respect to λ reads

$$\left\langle \delta \lambda, p - c^{-1} \frac{d\xi}{ds} \right\rangle = 0 \quad \forall \delta \lambda \in T_\lambda \Lambda,$$

which we denote by

$$p = \mathbb{P}_{\mathcal{P}} \left(c^{-1} \frac{d\xi}{ds} \right).$$

The trajectory is then determined by stationarity with respect to ξ :

$$c \frac{\partial L}{\partial q} \cdot \delta\xi = - \left\langle \lambda, \frac{d\delta\xi}{ds} \right\rangle = - \left\langle \mathbb{P}_{\Lambda} \left(\frac{\partial L}{\partial \dot{q}} \right), \frac{d\delta\xi}{ds} \right\rangle \quad \forall \delta\xi \in T_{\xi}Q, \quad (19)$$

hence after time integration by parts,

$$\frac{1}{c} \frac{d}{ds} \mathbb{P}_{\Lambda} \left(\frac{\partial L}{\partial \dot{q}} \right) = \frac{\partial L}{\partial q},$$

which is the Euler-Lagrange equation in which we recognize the special time derivative $c^{-1}d\Box/ds$ equivalent to $d\Box/dt$ due to time reparametrization, and the projection \mathbb{P}_{Λ} due to the introduction of the present mixed formulation.

Stationarity with respect to τ brings a redundant information on energy conservation:

$$\int_0^S c \frac{\partial L}{\partial t} \cdot \delta\tau + L \frac{d\delta\tau}{ds} - \langle \lambda, p \rangle \frac{d\delta\tau}{ds} = 0 \quad \forall \delta\tau,$$

whereby :

$$\frac{1}{c} \frac{d}{ds} (\langle \lambda, p \rangle - L) = - \frac{\partial L}{\partial t}.$$

The Hamilton function of the system is therefore:

$$H = \langle \lambda, p \rangle - L = \left\langle \mathbb{P}_{\Lambda} \left(\frac{\partial L}{\partial \dot{q}} \right), p \right\rangle - L \quad (20)$$

$$= \left\langle \mathbb{P}_{\Lambda} \left(\frac{\partial L}{\partial \dot{q}} \right), \frac{1}{c} \frac{d\xi}{ds} \right\rangle - L. \quad (21)$$

This is also obtained from (19) by using the test function $\delta\xi = \dot{q} = c^{-1}d\xi/ds$. Nevertheless, in the discrete framework, this additional equation can be used to conciliate energy conservation and symplecticity.

In addition, we get:

Theorem 3 (Symplecticity) *For every $s \in [0, S]$, define the skew symmetric bilinear form:*

$$\omega(s; d_1X(s), d_2X(s)) = \frac{\partial^2 L}{\partial \dot{q}^2}(X(s)) d_2p \wedge \mathbb{P}_{\mathcal{P}} d_1\xi + \frac{\partial^2 L}{\partial \dot{q} \partial q}(X(s)) d_2\xi \wedge \mathbb{P}_{\mathcal{P}} d_1\xi,$$

for every $d_1\xi, d_2\xi \in T_{\xi(s)}Q$ and every $d_2p \in T_{p(s)}P$. The variations of the solution $X(s) = (\xi(s), p(s))$ are tied by the following relationship

$$\omega(0; d_1X(0), d_2X(0)) = \omega(s; d_1X(s), d_2X(s)), \quad \forall s \in [0, S].$$

Proof. We differentiate the action in the vicinity of a trajectory, and make use of the stationarity conditions. The only remaining terms are the one accounting for the initial and final conditions of the trajectory. It follows that

$$d\mathfrak{S} = [\langle \lambda, d\xi \rangle]_0^S = \left[\left\langle \frac{\partial L}{\partial \dot{q}}, \mathbb{P}_{\mathcal{P}} d\xi \right\rangle \right]_0^S.$$

Since the second derivative is symmetric, or in the sense of differential forms $d^2\mathfrak{S} = 0$, we get:

$$0 = \left[\frac{\partial^2 L}{\partial \dot{q}^2} d_2 p \wedge \mathbb{P}_{\mathcal{P}} d_1 \xi + \frac{\partial^2 L}{\partial \dot{q} \partial q} d_2 \xi \wedge \mathbb{P}_{\mathcal{P}} d_1 \xi \right]_0^S, \quad \forall d_1 \xi, d_2 \xi \in T_{\xi} Q, \quad \forall d_2 p \in T_p P.$$

Hence the announced conservation.

We turn now to the analysis of symmetries and conservation. Let (ξ, τ) be a trajectory of the system; we denote by $\mathbb{S}(\xi, \tau) = \mathfrak{S}(\xi, \tau, p, \lambda)$ the reduced action, where (p, λ) is the solution in velocities and Lagrange multipliers.

Let $R : \Theta \times Q \rightarrow Q$ be a transformation of the solution and Θ a group of symmetries, such that $R(\cdot, q)$ is a group morphism on Θ for every $q \in Q$. We assume that if q is solution, $R(\theta, q)$ is also a solution for every $\theta \in \Theta$. In other words,

$$\mathbb{S}(R(\theta, \xi), \tau) = \mathbb{S}(\xi, \tau) \quad \forall \theta \in \Theta.$$

Theorem 4 (Noether's theorem) *Under the previous assumptions, the following quantity:*

$$\left\langle \mathbb{P}_{\Lambda} \left(\frac{\partial L}{\partial \dot{q}} \right), \frac{\partial R}{\partial \theta}(0, q) \right\rangle$$

is conserved along the dynamics.

Proof. Since

$$\mathbb{S}(R(\theta, \xi), \tau) = \mathbb{S}(\xi, \tau) \quad \forall \theta \in \Theta,$$

the differential of $\mathbb{S}(R(\theta, \xi), \tau)$ with respect to θ vanishes. After integration by parts in time, it follows that for the solution (ξ, τ) ,

$$\left[\left\langle \mathbb{P}_{\Lambda} \left(\frac{\partial L}{\partial \dot{q}} \right), \frac{\partial R}{\partial \theta}(0, \xi) \right\rangle \right]_0^S = 0,$$

which is the announced result.

Remark 8 *The above Noether's theorem could be easily extended to the case of a symmetry group over time. As a consequence, energy conservation appears as a simple consequence of the invariance of the Lagrange function with respect to time.*

2.4.2 Discrete counterpart

Discrete variational time integrators are based upon the same variational principle as the continuous case above, but rely on a discrete version of the Lagrange function. Let us denote by (q_n) and (p_n) the values of q and p approximated at discrete times (t_n) . A discrete version of the Lagrange function can be formulated as:

$$\mathfrak{S}_h((q_n), (p_n), (t_n)) = \sum_{n=0}^N L_h(q_n, q_{n+1}, p_n, p_{n+1}, t_n, t_{n+1}) - \langle \lambda_n, B_h(q_n, q_{n+1}, p_n, p_{n+1}, t_n, t_{n+1}) \rangle,$$

where B_h is a linear constraint operator; q_0 and q_{N+1} are assumed to be known.

Denoting by $(q_0, q_1, p_0, p_1, t_0, t_1)$ the generic arguments of L_h and B_h , and by $X_n = (q_n, q_{n+1}, p_n, p_{n+1}, t_n, t_{n+1})$ the state vectors, the stationarity of the Lagrange function reads:

$$\left[\frac{\partial L_h}{\partial q_0}(X_{n+1}) + \frac{\partial L_h}{\partial q_1}(X_n) \right] \cdot \delta q_{n+1} - \left\langle \lambda_n, \frac{\partial B_h}{\partial q_1}(X_n) \cdot \delta q_{n+1} \right\rangle - \left\langle \lambda_{n+1}, \frac{\partial B_h}{\partial q_0}(X_{n+1}) \cdot \delta q_{n+1} \right\rangle = 0,$$

$$\left[\frac{\partial L_h}{\partial p_0}(X_{n+1}) + \frac{\partial L_h}{\partial p_1}(X_n) \right] \cdot \delta p_{n+1} - \left\langle \lambda_n, \frac{\partial B_h}{\partial p_1}(X_n) \cdot \delta p_{n+1} \right\rangle - \left\langle \lambda_{n+1}, \frac{\partial B_h}{\partial p_0}(X_{n+1}) \cdot \delta p_{n+1} \right\rangle = 0,$$

for every $0 \leq n \leq N-1$, every δq_{n+1} , δp_{n+1} and for every $0 \leq n \leq N$ and every $\delta \lambda_n$,

$$\langle \delta \lambda_n, B_h(X_n) \rangle = 0.$$

Stationarity with respect to the time variables implies

$$\left[\frac{\partial L_h}{\partial t_0}(X_{n+1}) + \frac{\partial L_h}{\partial t_1}(X_n) \right] \cdot \delta t_{n+1} - \left\langle \lambda_n, \frac{\partial B_h}{\partial t_1}(X_n) \cdot \delta t_{n+1} \right\rangle - \left\langle \lambda_{n+1}, \frac{\partial B_h}{\partial t_0}(X_{n+1}) \cdot \delta t_{n+1} \right\rangle = 0,$$

for every δt_{n+1} . Additionally, one has to take into account the initial and final conditions:

$$\frac{\partial L_h}{\partial p_0}(X_0) \cdot \delta p_0 - \left\langle \lambda_0, \frac{\partial B_h}{\partial p_0}(X_0) \cdot \delta p_0 \right\rangle = 0, \quad \forall \delta p_0.$$

$$\frac{\partial L_h}{\partial p_1}(X_N) \cdot \delta p_{N+1} - \left\langle \lambda_N, \frac{\partial B_h}{\partial p_1}(X_N) \cdot \delta p_{N+1} \right\rangle = 0, \quad \forall \delta p_{N+1}.$$

We assume that at least one of the operators $\frac{\partial B_h^\top}{\partial p_0}(X_0)$ or $\frac{\partial B_h^\top}{\partial p_1}(X_N)$ is invertible.

Let us assume for the present development that $\frac{\partial B_h^\top}{\partial p_0}(X_0)$ is invertible. In this case, one has:

$$\lambda_0 = \frac{\partial B_h^{-\top}}{\partial p_0}(X_0) \frac{\partial L_h}{\partial p_0}(X_0).$$

In case $\frac{\partial B_h^\top}{\partial p_1}(X_N)$ is invertible, one may use in the foregoing proofs that

$$\lambda_N = \frac{\partial B_h^{-\top}}{\partial p_1}(X_N) \frac{\partial L_h}{\partial p_1}(X_N)$$

and similar arguments.

Theorem 5 (Symplecticity) *The resulting time integration scheme is symplectic.*

Proof. By differentiation of the discrete action and taking into account the stationarity conditions, one gets

$$\begin{aligned} d\mathfrak{S}_h &= \frac{\partial L_h}{\partial q_0}(X_0) \cdot \delta q_0 - \left\langle \lambda_0, \frac{\partial B_h}{\partial q_0}(X_0) \cdot \delta q_0 \right\rangle \\ &\quad + \frac{\partial L_h}{\partial q_1}(X_N) \cdot \delta q_{N+1} - \left\langle \lambda_N, \frac{\partial B_h}{\partial q_1}(X_N) \cdot \delta q_{N+1} \right\rangle \\ &= \frac{\partial L_h}{\partial q_0}(X_0) \cdot \delta q_0 - \left\langle \lambda_0, \frac{\partial B_h}{\partial q_0}(X_0) \cdot \delta q_0 \right\rangle \\ &\quad - \frac{\partial L_h}{\partial q_0}(X_{N+1}) \cdot \delta q_{N+1} + \left\langle \lambda_{N+1}, \frac{\partial B_h}{\partial q_0}(X_{N+1}) \cdot \delta q_{N+1} \right\rangle \\ &= \frac{\partial L_h}{\partial q_0}(X_0) \cdot \delta q_0 - \left\langle \frac{\partial L_h}{\partial p_0}(X_0), \frac{\partial B_h^{-1}}{\partial p_0}(X_0) \frac{\partial B_h}{\partial q_0}(X_0) \cdot \delta q_0 \right\rangle \\ &\quad - \frac{\partial L_h}{\partial q_0}(X_{N+1}) \cdot \delta q_{N+1} + \left\langle \frac{\partial L_h}{\partial p_0}(X_{N+1}), \frac{\partial B_h^{-1}}{\partial p_0}(X_{N+1}) \frac{\partial B_h}{\partial q_0}(X_{N+1}) \cdot \delta q_{N+1} \right\rangle \\ &= A(X_0) \cdot \delta q_0 - A(X_{N+1}) \cdot \delta q_{N+1}, \end{aligned}$$

in which the generalized linear momentum is defined as

$$A(X_n) = \frac{\partial L_h}{\partial q_0}(X_n) - \frac{\partial B_h^\top}{\partial q_0} \frac{\partial B_h^{-\top}}{\partial p_0} \frac{\partial L_h}{\partial p_0}(X_n).$$

The announced result follows by additional differentiation.

Proceeding exactly as in the continuous case, the discrete Noether's theorem reads:

Theorem 6 *For every $n \geq 0$,*

$$A(X_n) \cdot \frac{\partial R}{\partial \theta}(0, q_n) = A(X_0) \cdot \frac{\partial R}{\partial \theta}(0, q_0).$$

Good energy evolution properties follows from symplecticity (cf. [13]). In case

of discrete time reparametrization, exact conservation will be obtained provided the equation on the time step remains solvable.

2.4.3 Newmark scheme

We exemplify herein the design of mixed variational integrators on a simple example. Let us consider the following discrete action:

$$S((\varphi_n), (p_n), (\lambda_n), (t_n)) = \sum_{n=0}^N \frac{t_{n+1} - t_n}{2} \int_{\Omega} \varrho |p_{n+1}|^2 - (t_{n+1} - t_n) \int_{\Omega} W(\nabla \varphi_{n+1}) - (t_{n+1} - t_n) \int_{\Omega} \lambda_{n+1} \cdot \left(\frac{p_n + p_{n+1}}{2} - \frac{\varphi_{n+1} - \varphi_n}{t_{n+1} - t_n} \right).$$

Stationnarization with respect to (p_n) implies for all variations (δp_n) ,

$$\Delta t_n \int_{\Omega} \varrho p_n \cdot \delta p_n - \int_{\Omega} \frac{\Delta t_n \lambda_n + \Delta t_{n+1} \lambda_{n+1}}{2} \cdot \delta p_n = 0, \quad (22)$$

with $\Delta t_n = t_n - t_{n-1}$. Stationnarization with respect to (φ_n) implies for all variations $(\delta \varphi_n)$,

$$\int_{\Omega} \frac{\lambda_{n+2} - \lambda_{n+1}}{\Delta t_{n+1}} \cdot \delta \varphi_{n+1} + \int_{\Omega} \partial_F W(\nabla \varphi_{n+1}) : \nabla \delta \varphi_{n+1} = 0. \quad (23)$$

Stationnarization with respect to (λ_n) simply implies for all variations $(\delta \lambda_n)$, the displacements-velocities relationships

$$\int_{\Omega} \delta \lambda_{n+1} \cdot \left(\frac{p_n + p_{n+1}}{2} - \frac{\varphi_{n+1} - \varphi_n}{\Delta t_{n+1}} \right) = 0. \quad (24)$$

We now decide to reformulate the present scheme in a more tractable form by introducing the velocities $(\dot{\varphi}_n)$ and (ξ_n) such that

$$p_n = \mathbb{P}_{\mathcal{P}_h} \dot{\varphi}_n \quad \lambda_n = \mathbb{P}_{\Lambda_h}(\rho \xi_n),$$

with

$$\begin{cases} \frac{\Delta t_n \xi_n + \Delta t_{n+1} \xi_{n+1}}{2} = \Delta t_n \dot{\varphi}_n, \\ \frac{\dot{\varphi}_n + \dot{\varphi}_{n+1}}{2} = \frac{\varphi_{n+1} - \varphi_n}{\Delta t_{n+1}}. \end{cases} \quad (25)$$

Equation (23) then provides the following time integration scheme:

$$\begin{aligned} & \frac{1}{\Delta t_{n+1}} \int_{\Omega} \varrho \mathbb{P}_{\mathcal{P}_h} \left(4\nu_{n+1} \frac{\varphi_{n+1} - \varphi_n}{\Delta t_{n+1}} - 2\nu_{n+1} \dot{\varphi}_n - (1 + \nu_{n+1}) \xi_{n+1} \right) \cdot \mathbb{P}_{\mathcal{P}_h} \delta \varphi_{n+1} \\ & + \int_{\Omega} \partial_F W(\nabla \varphi_{n+1}) : \nabla \delta \varphi_{n+1} = 0, \end{aligned} \quad (26)$$

with $\nu_{n+1} = \Delta t_{n+1}/\Delta t_{n+2}$ and relationships (25) to get $\dot{\varphi}_{n+1}$ and ξ_{n+2} ; another time step Δt_{n+3} needs to be chosen for the next step.

Remark 9 *Assume the time step is constant and introduce*

$$\xi_{n+1} = \dot{\varphi}_n + \frac{\Delta t}{2} \ddot{\varphi}_n.$$

The scheme reduces to

$$\int_{\Omega} \varrho \mathbb{P}_{\mathcal{P}_h} \left(2 \frac{\dot{\varphi}_n - \dot{\varphi}_{n-1}}{t_n - t_{n-1}} - \ddot{\varphi}_{n-1} \right) \cdot \mathbb{P}_{\mathcal{P}_h} \delta \varphi_n + \int_{\Omega} \partial_F W(\nabla \varphi_n) : \nabla \delta \varphi_n = 0, \quad (27)$$

complemented by the relationships

$$\begin{cases} \frac{\ddot{\varphi}_n + \ddot{\varphi}_{n+1}}{2} = \frac{\dot{\varphi}_{n+1} - \dot{\varphi}_n}{t_{n+1} - t_n} \\ \frac{\dot{\varphi}_n + \dot{\varphi}_{n+1}}{2} = \frac{\varphi_{n+1} - \varphi_n}{t_{n+1} - t_n}. \end{cases} \quad (28)$$

This scheme is known to be part of the Newmark's schemes; cf [25], Kane et al. for a geometric analysis.

Remark 10 *We have demonstrated here that the derivation of variational schemes is made easier through the proposed mixed approach; it enables the independent choices for the displacements and velocities spaces, as well as the discrete time relationship between both.*

Let us now render the discrete action stationary with respect to the time discretization points (t_n) ; one gets the discrete version of the energy conservation principle $E_{n+1} = E_n$, where the discrete energy is given by

$$E_n = \frac{1}{2} \int_{\Omega} \varrho |p_n|^2 - \int_{\Omega} W(\nabla \varphi_n) - \int_{\Omega} \lambda_n \cdot \frac{p_{n-1} + p_n}{2}.$$

From the numerical point of view, two questions remain crucial. The solvability on the equation determining the sequence (t_n) , and the uniqueness of each discrete time. Clearly, uniqueness is not possible in general. Indeed, a midpoint scheme on a linear wave equation preserves energy exactly independently of the time step, which proves the non-uniqueness statement.

The question of existence remains more difficult in general.

3 Interpretation of the KLR approach

3.1 Mass lumping and strong persistency condition

Let $\Gamma_c \subset \partial\Omega$ be a part of the domain boundary potentially entering into contact with an external rigid obstacle. Considering a linearized kinematics for the displacements $u^h \in \Phi_h$, the contact condition expresses in the mortar sense [26]

$$\int_{\Gamma_c} \mu n \cdot u^h \leq \int_{\Gamma_c} \mu g \quad \forall \mu \in M_h^+,$$

where n is a regularized normal field over Γ_c and M_h^+ a space of positive Lagrange multipliers. The linearized dynamic equations in presence of contact consists of finding $u^h \in \Phi_h$ and $\mu^h \in M_h^+$ such that

$$\begin{cases} m(\mathbb{P}_{\mathcal{P}_h} \ddot{u}^h, \mathbb{P}_{\mathcal{P}_h} \delta u^h) + a(u^h, \delta u^h) = \ell(t; \delta u^h) + \int_{\Gamma_c} \mu^h n \cdot \delta u^h & \forall \delta u^h \in \Phi_{h,0}, \\ \int_{\Gamma_c} \delta \mu^h n \cdot u^h \leq \int_{\Gamma_c} \delta \mu^h g & \forall \delta \mu^h \in M_h^+, \\ \int_{\Gamma_c} \mu^h (u^h \cdot n - g) = 0, \end{cases} \quad (29)$$

where $\Phi_{h,0} = T_{u^h} \Phi_h$ is the vector space for displacements satisfying homogeneous boundary conditions.

We proceed with the introduction of the following decomposition of displacements:

$$\Phi_h = \mathring{\Phi}_h \oplus \bar{\Phi}_h,$$

where $\mathring{u}^h \in \mathring{\Phi}_h$ whenever

$$\int_{\Gamma_c} \mu^h n \cdot \mathring{u}^h = 0 \quad \forall \mu^h \in M_h^+.$$

In the sequel, we will assume $\mathbb{P}_{\mathcal{P}_h} \bar{\Phi}_h = 0$ or equivalently

$$\int_{\Omega} \lambda^h \cdot \bar{u}^h = 0 \quad \forall \lambda^h \in \Lambda^h, \forall \bar{u}^h \in \bar{\Phi}_h.$$

As a consequence, system (29) decouples into

$$\begin{cases} m \left(\mathbb{P}_{\mathcal{P}_h} \frac{\partial^2}{\partial t^2} \dot{u}^h, \mathbb{P}_{\mathcal{P}_h} \delta \dot{u}^h \right) + a(\bar{u}^h, \delta \dot{u}^h) + a(\dot{u}^h, \delta \dot{u}^h) = \ell(t; \delta \dot{u}^h) & \forall \delta \dot{u}^h \in \dot{\Phi}_{h,0}, \\ a(\dot{u}^h, \delta \bar{u}^h) + a(\bar{u}^h, \delta \bar{u}^h) = \ell(t; \delta \bar{u}^h) + \int_{\Gamma_c} \mu^h n \cdot \delta \bar{u}^h & \forall \delta \bar{u}^h \in \bar{\Phi}_{h,0}, \\ \int_{\Gamma_c} \delta \mu^h n \cdot \bar{u}^h \leq \int_{\Gamma_c} \delta \mu^h g & \forall \delta \mu^h \in M_h^+, \\ \int_{\Gamma_c} \mu^h (\bar{u}^h \cdot n - g) = 0, \end{cases} \quad (30)$$

i.e. a dynamical problem without contact and a static problem with contact. This key idea results into the following powerful result.

Theorem 7 *Assuming $\mathbb{P}_{\mathcal{P}_h} \bar{\Phi}_h = 0$, there exists a Lipschitz solution in time to (29). Additionally, the following persistency condition holds,*

$$\int_{\Gamma_c} \mu^h n \cdot \dot{u}^h = 0 \quad \text{on } [0, T],$$

from which energy conservation is achieved, i.e. for all $t \geq 0$,

$$\begin{aligned} & \frac{1}{2} m(\mathbb{P}_{\mathcal{P}_h} \dot{u}(t), \mathbb{P}_{\mathcal{P}_h} \dot{u}(t)) + \frac{1}{2} a(u(t), u(t)) \\ &= \frac{1}{2} m(\mathbb{P}_{\mathcal{P}_h} \dot{u}(0), \mathbb{P}_{\mathcal{P}_h} \dot{u}(0)) + \frac{1}{2} a(u(0), u(0)) + \int_0^t \ell(s; \dot{u}(s)) ds. \end{aligned} \quad (31)$$

Proof. The proof exactly follows the arguments of Khenous, Laborde and Renard [18,38]. In system (30), \bar{u}^h is uniquely defined as soon as \dot{u}^h is known; $\bar{u}^h \in \mathcal{K}^h$ such that

$$a(\bar{u}^h, \bar{w}^h - \bar{u}^h) \geq \ell(t; \bar{w}^h - \bar{u}^h) - a(\dot{u}^h, \bar{w}^h - \bar{u}^h) \quad \forall \bar{w}^h \in \mathcal{K}^h,$$

where

$$\mathcal{K}^h = \left\{ \bar{w}^h \in \bar{\Phi}^h, \int_{\Gamma_c} \delta \mu^h \cdot (\bar{w}^h \cdot n) \leq \int_{\Gamma_c} \delta \mu^h \cdot g \quad \forall \delta \mu^h \in M_h^+ \right\}.$$

We denote $\bar{u}^h = \mathcal{B}(\dot{u}^h)$, where $\mathcal{B} : \dot{\Phi}_h \rightarrow \bar{\Phi}_h$ is Lipschitz continuous. Namely, for every \dot{u}_1^h and $\dot{u}_2^h \in \mathcal{K}^h$,

$$\|\mathcal{B}(\dot{u}_2^h) - \mathcal{B}(\dot{u}_1^h)\|_a \leq \|\dot{u}_2^h - \dot{u}_1^h\|_a, \quad (32)$$

where $\|\square\|_a = a(\square, \square)^{1/2}$.

It follows from system (30) that we finally have look for $\dot{u}^h \in \mathring{\Phi}_h$ such that

$$m \left(\mathbb{P}_{\mathcal{P}_h} \frac{\partial^2}{\partial t^2} \dot{u}^h, \mathbb{P}_{\mathcal{P}_h} \delta \dot{u}^h \right) = \ell(t; \delta \dot{u}^h) - a(\mathcal{B}(\dot{u}^h), \delta \dot{u}^h) - a(\dot{u}^h, \delta \dot{u}^h) \quad \forall \delta \dot{u}^h \in \mathring{\Phi}_{h,0}.$$

This is an ordinary differential equation with Lipschitz right-hand side. It admits a solution $\dot{u}^h \in C^2(0, T; \mathring{\Phi}^h)$.

As in [18], one gets $\mu^h \in W^{1,\infty}(0, T; M_h)$ and

$$\int_{\Gamma_c} \mu^h n \cdot \dot{u}^h = 0$$

from the regularity of the solution. Energy conservation follows from using the test function $\delta u^h = \dot{u}^h$ in the equation of the dynamics.

3.2 Some choices of spaces

We proceed with several admissible choices of spaces. First observe that independently of the choice of M_h , one gets

$$\bar{\Phi}_h \subset \bar{\Phi}_h^{max} = \text{span}\{\psi_i, i \in \bar{I}\}^3,$$

where $(\psi_i)_{i \in I}$ are the scalar shape functions associated to the displacements in Φ_h and the subset \mathring{I} is such that $\psi_i = 0$ on Γ_c for all $i \in \mathring{I}$; we have denoted $\bar{I} = I \setminus \mathring{I}$. Let us propose here three spaces Φ_h , \mathcal{P}_h and Λ_h such that

$$\mathbb{P}_{\mathcal{P}_h} \bar{\Phi}_h^{max} = 0.$$

We restrict ourself here to linear displacements with linear or constant velocities but the reader will recognize a number of possibilities satisfying the key-assumptions. As examples let us mention

- bubble enrichment of the proposed linear displacements with the same velocity spaces and Lagrange multipliers,
- quadratic displacements with quadratic velocities, continuous or discontinuous linear velocities.

Remark 11 *Observe that to preserve the transfer of linear momentum – and therefore to trigger tangential waves – on the contact interface, the mass action should only be modified along the normal direction.*

3.2.1 Linear displacements, modified linear velocities

Starting from the standard \mathbb{P}_1 or \mathbb{Q}_1 approximation for displacements,

$$\Phi_h = \text{span}\{\psi_i, i \in I\}^3,$$

let us define a modified basis $(\mathring{\psi}_j)_{j \in \mathring{I}}$ for $\mathcal{P}_h = \text{span}\{\mathring{\psi}_j, j \in \mathring{I}\}^3$, such that

$$\mathring{\psi}_j = \psi_j + \sum_{k \in \bar{I}} \alpha_j^k \psi_k \quad \text{with} \quad \sum_{j \in \mathring{I}} \alpha_j^k = 1 \text{ for all } k \in \bar{I}.$$

Using such a space, the approximation property of \mathcal{P}_h is optimal. Let us now define the dual basis $(\psi_i^*)_{i \in I}$ such that

$$\int_{\Omega} \psi_i \psi_j^* = \delta_{ij}$$

where δ_{ij} is the Krönecker symbol. Let us now define

$$\Lambda_h = \text{span}\{\psi_j^*, j \in \mathring{I}\}^3.$$

It follows that for every $\varphi \in \bar{\Phi}_h^{\max}$ and every $\lambda \in \Lambda_h$,

$$\int_{\Omega} \varphi \cdot \lambda = 0,$$

from which

$$\mathbb{P}_{\mathcal{P}_h} \bar{\Phi}_h^{\max} = 0.$$

Let us finally prove the inf-sup condition for the chosen spaces:

Theorem 8 *The inf-sup condition (2) is satisfied.*

Proof. Let us first introduce the operator $\pi_h : L^2(\Omega)^3 \rightarrow \mathcal{P}_h$ such that for every $p \in L^2(\Omega)^3$,

$$\int_{\Omega} (\pi_h p) \cdot \lambda_h = \int_{\Omega} p \cdot \lambda_h \quad \forall \lambda_h \in \Lambda_h.$$

It follows from the above definitions that

$$\pi_h p = \sum_{i \in \mathring{I}} \mathring{\psi}_i \int_{\Omega} p \psi_i^*,$$

and one gets the estimate:

$$\|\pi_h p\|_{L^2(\Omega)^3}^2 \leq \sum_{i \in \mathring{I}} \|p\|_{L^2(K_i)^3}^2 \|\psi_i^*\|_{L^2(K_i)^3}^2 \|\mathring{\psi}_i\|_{L^2(K_i)^3}^2 \leq C \|p\|_{L^2(\Omega)^3}^2,$$

where K_i is the support of the shape function ψ_i . Assuming regularity of the mesh, the last inequality can be easily proven by a change of variable onto

reference elements. The stability of the operator π_h classically establishes the inf-sup condition (2).

3.3 Linear displacements; piecewise constant velocities

Using the same discretization of the displacements as above, we propose the use of piecewise constant velocity fields, i.e.

$$\mathcal{P}_h = \text{span}\{1_K, K \in \mathcal{K}_h\}^3,$$

where 1_A is the function taking the value 1 over the set A and 0 elsewhere; \mathcal{K}_h is the mesh of Ω . This space provides the optimal approximation property required for \mathcal{P}_h .

We now define

$$\Lambda_h = \text{span}\{1_K \theta_K, K \in \mathcal{K}_h\}^3$$

with for all $K \in \mathcal{K}_h$,

$$\int_K \theta_K = 1 \quad \text{and} \quad \int_K \theta_K \psi_i = 0 \quad \forall i \in \bar{I}.$$

from which $\mathbb{P}_{\mathcal{P}_h} \bar{\Phi}_h^{max} = 0$. The proof of the inf-sup condition (2) follows the same lines as for Theorem 8.

Theorem 9 *The inf-sup condition (2) is satisfied.*

4 Numerical tests

4.1 Numerical choices

4.1.1 Mass lumping

We validate herein the approach detailed in Section 3.2.1 with the specific choice

$$\alpha_j^k = \frac{|X_j - X_k|}{\sum_{\ell \in \bar{I}} |X_\ell - X_k|},$$

$(X_i)_{i \in I}$ being the positions of the nodes of the mesh respectively associated with the Lagrange shape functions $(\psi_i)_{i \in I}$. It results into a velocity space almost identical to the displacements space, except in the neighborhood of the contact zone. The authors have proposed this simple choice in [41]. It enables the conservation of the total mass of the system; some other approaches also

propose conservation of the inertia tensor like [17,18,12], but since geometry approximation already introduces such modification for industrial structures, we will stick to the present much simpler modification.

4.1.2 Kinematical constraints and discretization

The following test cases have been discretized in space using bilinear \mathbb{Q}_1 hexahedron. Incompressibility has been additionally enforced against piecewise constant \mathbb{Q}_0 hydrostatic pressures in penalized form, namely adding the energy

$$\frac{1}{2}G \sum_{E \in \mathcal{E}_h} \left(\int_E \det F \right)^2,$$

where the sum is over the mesh elements. Of course, the underlying $\mathbb{Q}_1/\mathbb{Q}_0$ formulation in displacements / hydrostatic pressures is well-known not to pass the inf-sup condition but remains very acceptable for many applications.

Frictionless contact has been implemented in the form of a pointwise penalization, namely

$$\frac{1}{2}K \sum_{N \in \mathcal{N}_h^c} S_N \left(g_N^+ \right)^2,$$

where the sum is over the nodes possibly in contact, g_N is the gap function at such nodes, g_N^+ (which is equal to g_N if $g_N > 0$, 0 otherwise) its positive part; S_N is a surface associated to node N such that $\sum_{N \in \mathcal{N}_h^c} S_N = |\Gamma_c|$.

4.1.3 Time integration schemes

The various time integration schemes mentioned in the paper are the following.

- (1) Two first order schemes, known to be linearly dissipative:
 - The Euler scheme presented in equation (13) applied to the non-linear problem, i.e.

$$\begin{cases} \int_{\Omega} \varrho \mathbb{P}_{\mathcal{P}} \frac{\dot{\varphi}_{n+1} - \dot{\varphi}_n}{\Delta t} \cdot \mathbb{P}_{\mathcal{P}} \delta \varphi + \int_{\Omega} \partial_F W(\nabla \varphi_{n+1}) : \nabla \delta \varphi = 0 & \forall \delta \varphi \in T_{\varphi} \Phi, \\ \dot{\varphi}_{n+1} = \frac{1}{\Delta t} (\varphi_{n+1} - \varphi_n). \end{cases} \quad (33)$$

- A *Euler-Newmark* scheme in which

$$\begin{cases} \int_{\Omega} \varrho \mathbb{P}_{\mathcal{P}} \frac{\dot{\varphi}_{n+1} - \dot{\varphi}_n}{\Delta t} \cdot \mathbb{P}_{\mathcal{P}} \delta \varphi + \int_{\Omega} \partial_F W(\nabla \varphi_{n+1}) : \nabla \delta \varphi = 0 & \forall \delta \varphi \in T_{\varphi} \Phi, \\ \frac{1}{2} (\dot{\varphi}_n + \dot{\varphi}_{n+1}) = \frac{1}{\Delta t} (\varphi_{n+1} - \varphi_n). \end{cases} \quad (34)$$

(2) Two symplectic integrators:

- The first order symplectic Newmark scheme derived in section 2.4.3,
- The second order midpoint scheme

$$\begin{cases} \int_{\Omega} \varrho \mathbb{P}_{\mathcal{P}} \frac{\dot{\varphi}_{n+1} - \dot{\varphi}_n}{\Delta t} \cdot \mathbb{P}_{\mathcal{P}} \delta\varphi + \int_{\Omega} \partial_F W(\nabla\varphi_{n+1/2}) : \nabla\delta\varphi = 0 & \forall \delta\varphi \in T_{\varphi}\Phi, \\ \frac{1}{2}(\dot{\varphi}_n + \dot{\varphi}_{n+1}) = \frac{1}{\Delta t}(\varphi_{n+1} - \varphi_n), \end{cases} \quad (35)$$

where $\varphi_{n+1/2} = \frac{1}{2}(\varphi_n + \varphi_{n+1})$.

(3) The conservative scheme introduced equation (11). In order to improve its performance in presence of frictionless contact, it is possible to use the modification proposed in [11,15]. Instead of the standard virtual work at mid-time,

$$\sum_{N \in \mathcal{N}_h^c} S_N \pi_N n_N \cdot \delta\varphi,$$

with $\pi_N = K g_N(\varphi_{n+1/2})^+$ and $n_N = \partial_{\varphi} g_N(\varphi_{n+1/2})$, we adopt

$$\begin{aligned} \pi_N^* &= K g_N(\varphi_{n+1/2})^+ + \\ &+ K \left[\frac{1}{2} |g_N(\varphi_{n+1})^+|^2 - \frac{1}{2} |g_N(\varphi_n)^+|^2 - g_N(\varphi_{n+1/2})^+ \Delta g_N \right] \frac{\Delta g_N}{|\Delta g_N|^2}, \end{aligned}$$

$$\begin{aligned} n_N^* &= \partial_{\varphi} g_N(\varphi_{n+1/2}) + \\ &+ \left[g_N(\varphi_{n+1}) - g_N(\varphi_n) - g_N(\varphi_{n+1/2}) \Delta\varphi_N \right] \frac{\Delta\varphi_N}{|\Delta\varphi_N|^2}, \end{aligned}$$

with $\Delta g_N = g_N(\varphi_{n+1}) - g_N(\varphi_n)$ and $\Delta\varphi_N = \varphi_{n+1}(N) - \varphi_n(N)$. It results into the exact conservation of energy in presence of frictionless contact. This last time integration scheme has not been tested herein; see [15] for a discussion. The interest of such a scheme in presence of mass redistribution has been presented in [12]; energy-conservation obviously holds, but is complemented by an increased regularity of the contact pressures.

4.2 Frictionless impact of a cube

To discuss the properties of the proposed approach, let us first consider a rubber cube of dimension $a = 0.01 \text{ m}$ impacting a plane wall at speed $V = 2.8 \text{ m/s}$. The material is modeled using a Mooney Rivlin law

$$W(F) = C_1 |F|^2 + C_2 |\text{cof } F|^2 + G |\det F - 1|^2,$$

with $C_1 = 0.65 \text{ MPa}$, $C_2 = 0.07 \text{ MPa}$, the bulk modulus $G = 1 \text{ GPa}$ with density $\varrho = 1120 \text{ kg/m}^3$. The frictionless contact constraint is penalized with a $K = 10^4 \text{ GPa}$ modulus.

A hexahedral mesh of size $h = 10^{-3}m$ is used and different time steps; typically $\Delta t = 5.10^{-5}s$ and $\Delta t = 10^{-5}s$.

The presented approach has been theoretically showed to enable the well-posedness of the linear semi-discrete approach. Its convergence – up to a sub-sequence – to the continuous problem in presence of a visco-elastic behavior with frictionless contact is established in [7]. We illustrate this improvement in regularity by representing the contact penalization energy in the nonlinear hyperelastic framework for the present simple case using the various schemes. It is shown on Figure 1, that not only this evolution exhibits smoothness, but also good behavior by time step refinement for all the presented schemes. On the contrary, the standard approach generates chaotic behaviors of the penalization energy and does not show any easily perceptible convergence. It is exemplified on Figure 2. Observe that even for the very dissipative implicit Euler scheme, the effect of the proposed approach is clear and fastens convergence to the continuous solution.

One may wonder if the smoothness of the contact penalization energy as a function of time remains independent of the coefficient K and if convergence is obtained as $K \rightarrow \infty$. Such energy reads

$$\int_{\Gamma_c} (Kg^+) g = \frac{1}{K} \int_{\Gamma_c} |Kg^+|^2,$$

and one would expect that the contact pressure $p = Kg^+$ converges as $K \rightarrow \infty$. Therefore, asymptotically for $K \rightarrow \infty$, the above integral would scale like K^{-1} . This is confirmed by Figure 3; multiplying K by 100, the contact penalization energy is indeed divided by 100 for the four schemes, which also shows pressures are properly converged. Additionally, the time evolution indeed retains the same smooth shape. This numerical proof establishes convergence of the pressure field as $K \rightarrow \infty$ and therefore the insensitivity of the approach with respect to the treatment of the constraint under penalized or mixed form.

To illustrate the improved regularity of the pressure field not only in time, but also in space, Figure 4 shows the pressure field at given times of the cube impact for $\Delta t = 5.10^{-5}s$ and the initial penalization. The comparison with the standard approach clearly pleads in favor of the present development.

Let us conclude this section by turning back to the big picture of energy conservation. For simplicity, the total discrete energy is always taken as

$$\mathfrak{E}_n = \frac{1}{2} \int_{\Omega} \varrho \dot{\varphi}_n^2 + \int_{\Omega} W(\nabla \varphi_n) + \frac{1}{2} G \sum_{E \in \mathcal{E}_h} \left(\int_E \det \nabla \varphi_n \right)^2 + \frac{1}{2} K \sum_{N \in \mathcal{N}_h^c} S_N \left(g_N(\varphi_n)^+ \right)^2,$$

even though each symplectic scheme provides an alternative expression converging to this one, up to term in Δt^p when achieving order p accuracy in

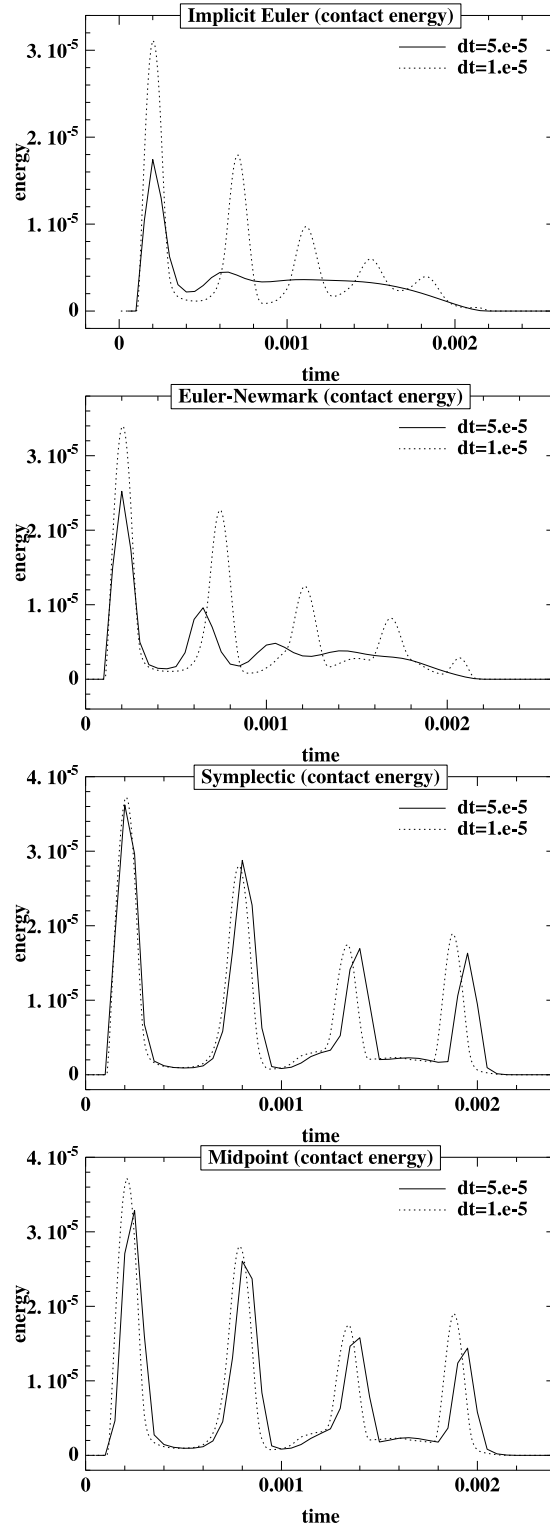


Fig. 1. Contact penalization energy with the proposed approach for the Implicit Euler, Euler-Newmark, the symplectic scheme from Section 2.4.3, and the symplectic Midpoint scheme using $\Delta t = 5 \cdot 10^{-5} s$ and $\Delta t = 10^{-5} s$. It illustrates both the smoothness in time of the energy, and its good behavior by time step refinement.

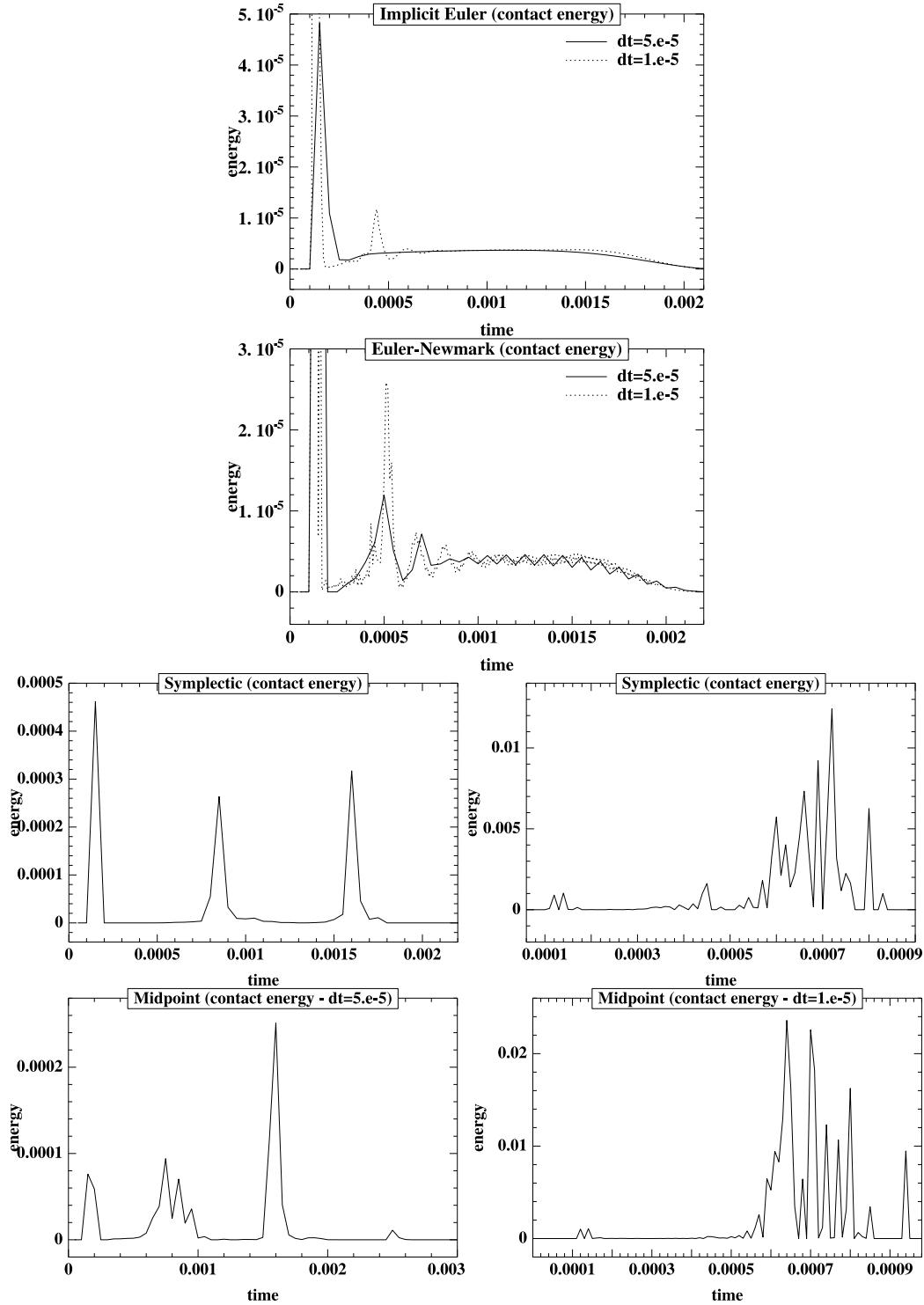


Fig. 2. Contact penalization energy with the standard approach for the Implicit Euler, Euler-Newmark, the symplectic scheme from Section 2.4.3, and the symplectic Midpoint scheme using $\Delta t = 5 \cdot 10^{-5} s$ (left column) and $\Delta t = 1 \cdot 10^{-5} s$ (right column). It illustrates the absence of convergence of the contact energy by time step refinement.

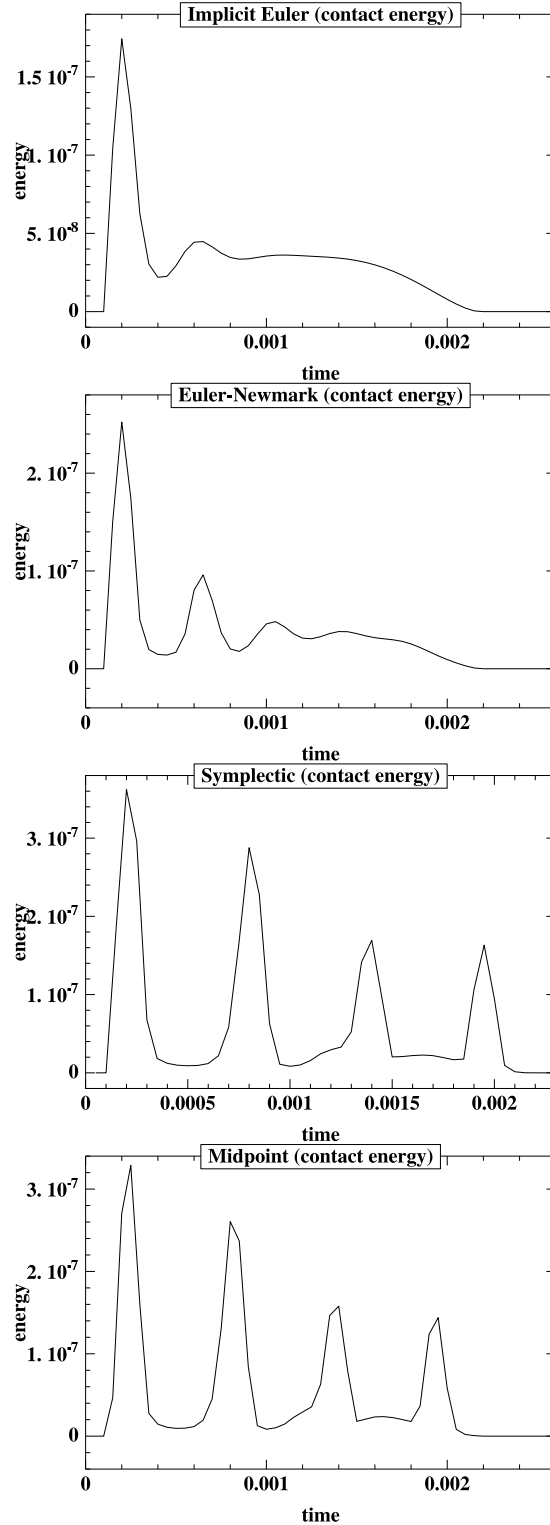


Fig. 3. Contact penalization energy with the proposed approach and the penalization coefficient $K = 10^6 GPa$ for the Implicit Euler, Euler-Newmark, the symplectic scheme from Section 2.4.3, and the symplectic Midpoint scheme using $\Delta t = 5 \cdot 10^{-5} s$. Compared with Figure 1, it illustrates the good behavior of the penalization contact energy as $K \rightarrow \infty$.

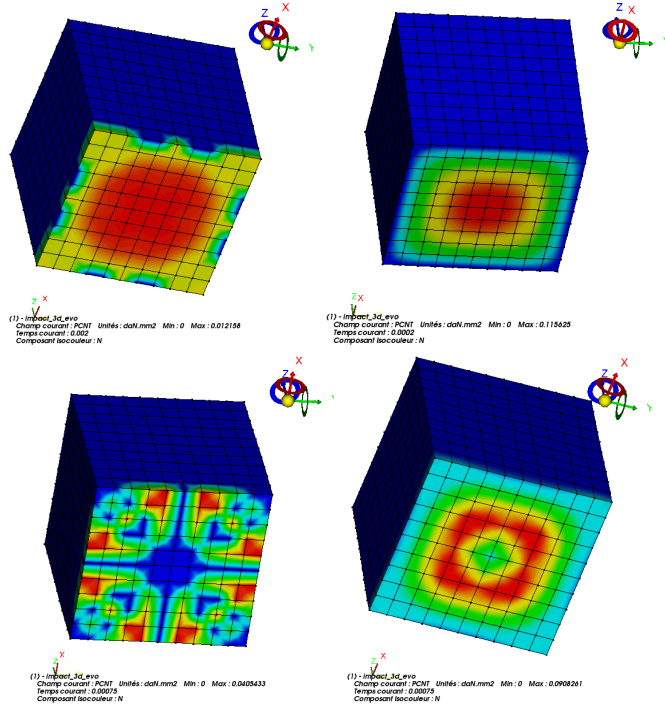


Fig. 4. Contact pressures for the Euler-Newmark scheme (upper line at $t = 0.002s$) and Symplectic scheme (lower line at $t = 0.0075s$) obtained with the proposed approach (right column) as compared to the standard technique (left column) using $\Delta t = 5.10^{-5}s$.

time. The only exception is made for the midpoint scheme where the subscript n is replaced by $n + 1/2$, particularly because the incompressibility and non-penetration constraints are chosen to be enforced at time $t_{n+1/2}$. Figures 5 and 6 show improved behavior of energy conservation using the present approach. It is particularly compelling in the case of the symplectic schemes, where excellent energy conservation is obtained with the present modification whereas oscillatory or accretive behavior can be observed when using a standard treatment of the frictionless contact constraint.

4.3 Impact of a sphere

Let us now turn to the case of a hollow sphere. This case is characterized by a less simple geometry and is more deformable to adapt itself to the contact zone.

The material, incompressibility and contact treatment are the same as in the previous section. The external and internal radii of the sphere are respectively $R_e = 0.25m$ and $R_i = 0.225m$; the impact speed is $V = 2.8m/s$.

We illustrate on Figure 8 the improved regularity in time of the contact penal-

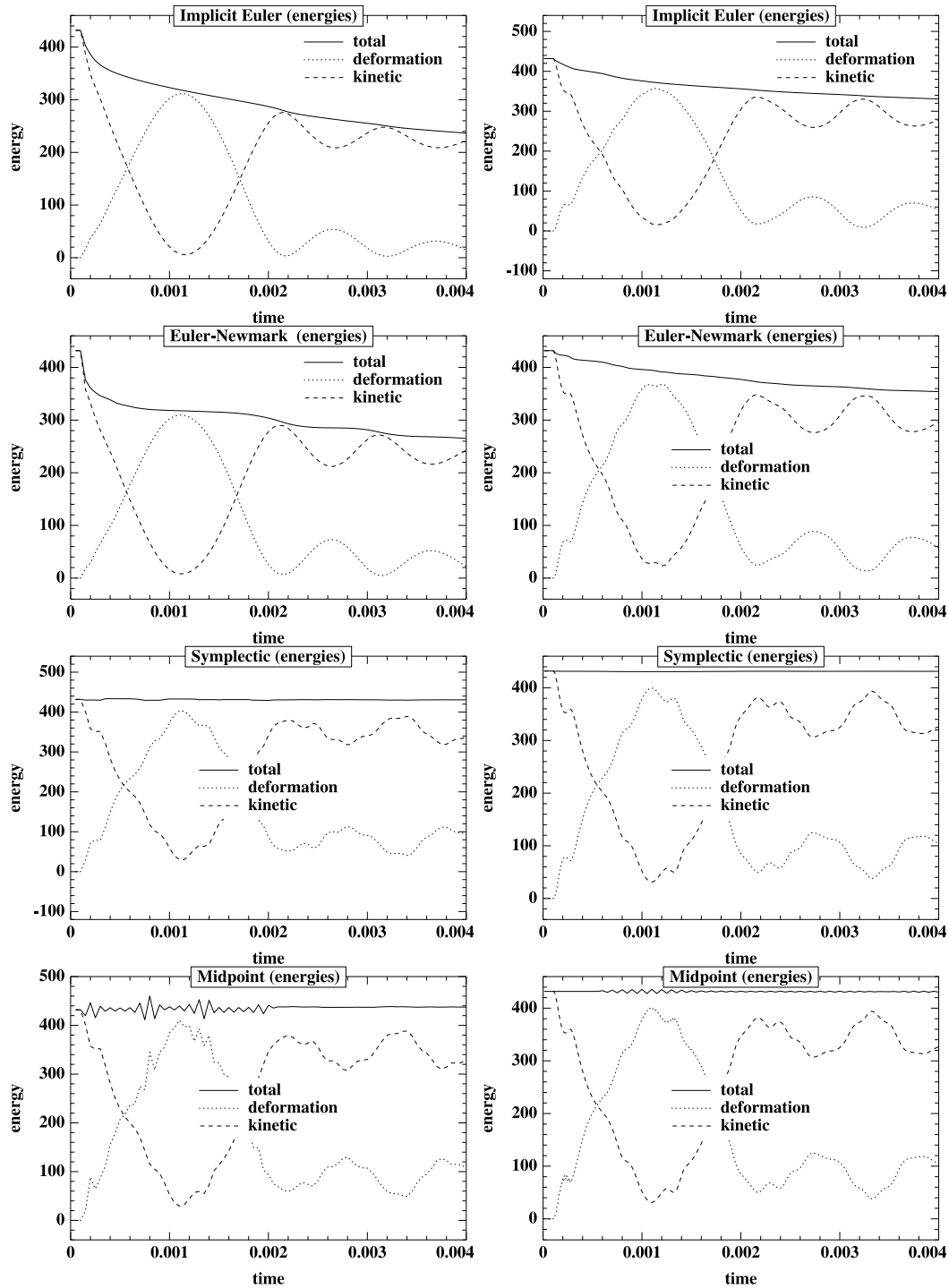


Fig. 5. Mechanical, kinetic and total energies with the proposed approach for the Implicit Euler, Euler-Newmark, the symplectic scheme from Section 2.4.3, and the symplectic Midpoint scheme using $\Delta t = 5.10^{-5}s$ (left column) and $\Delta t = 10^{-5}s$ (right column).

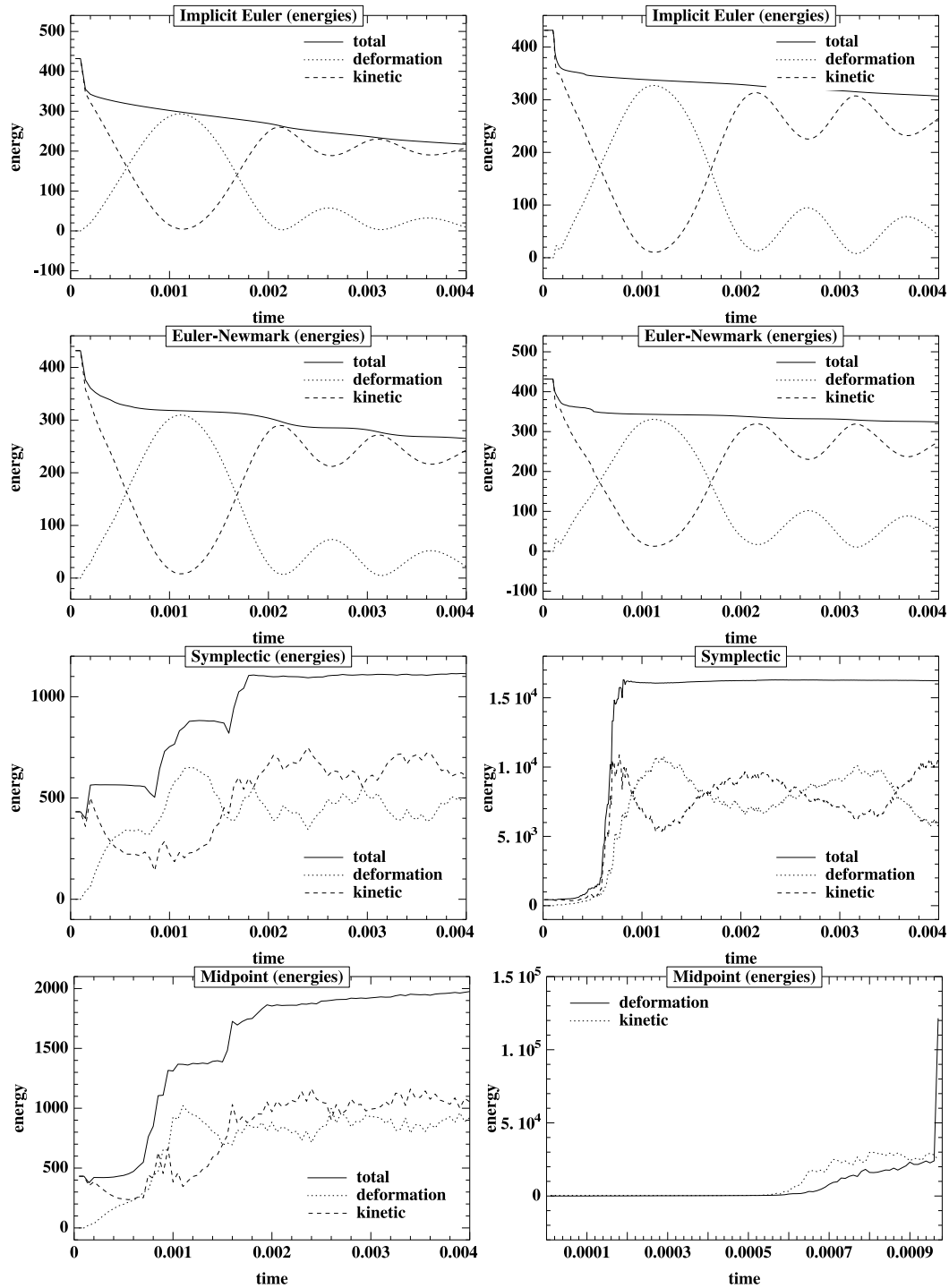


Fig. 6. Mechanical, kinetic and total energies with the standard approach for the Implicit Euler, Euler-Newmark, the symplectic scheme from Section 2.4.3, and the symplectic Midpoint scheme using $\Delta t = 5 \cdot 10^{-5} s$ (left column) and $\Delta t = 10^{-5} s$ (right column).

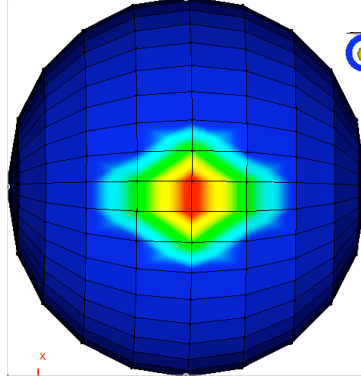


Fig. 7. Snapshot of the contact pressures of the ball when impacting the ground.

ization energy; for the standard approach, it is seen that the contact pressures do not converge by time step refinement since large oscillations in time of the penalization energy appear. Such oscillations are clearly avoided by mass redistribution.

Concerning energy evolution, it is clear from Figure 9 that the present approach clearly improves the conservation properties of the schemes, and in particular limit the accretive behavior of symplectic schemes during contact for large time steps.

5 Conclusion

In this paper, we have shown the flexibility and the potentialities of mixed time integration schemes in displacements and velocities 1) to enable the discrete well-posedness of contact problems and to identify various possible discretization schemes satisfying the right compatibility conditions between displacements and velocities, 2) to provide insensitive behavior of the time integration schemes with respect to the treatment of the non-penetration condition (strict or penalized), and 3) to extend the framework of variational integrators. In such a framework, the identification of the discrete energy balance could be used as a guideline for time step adaption.

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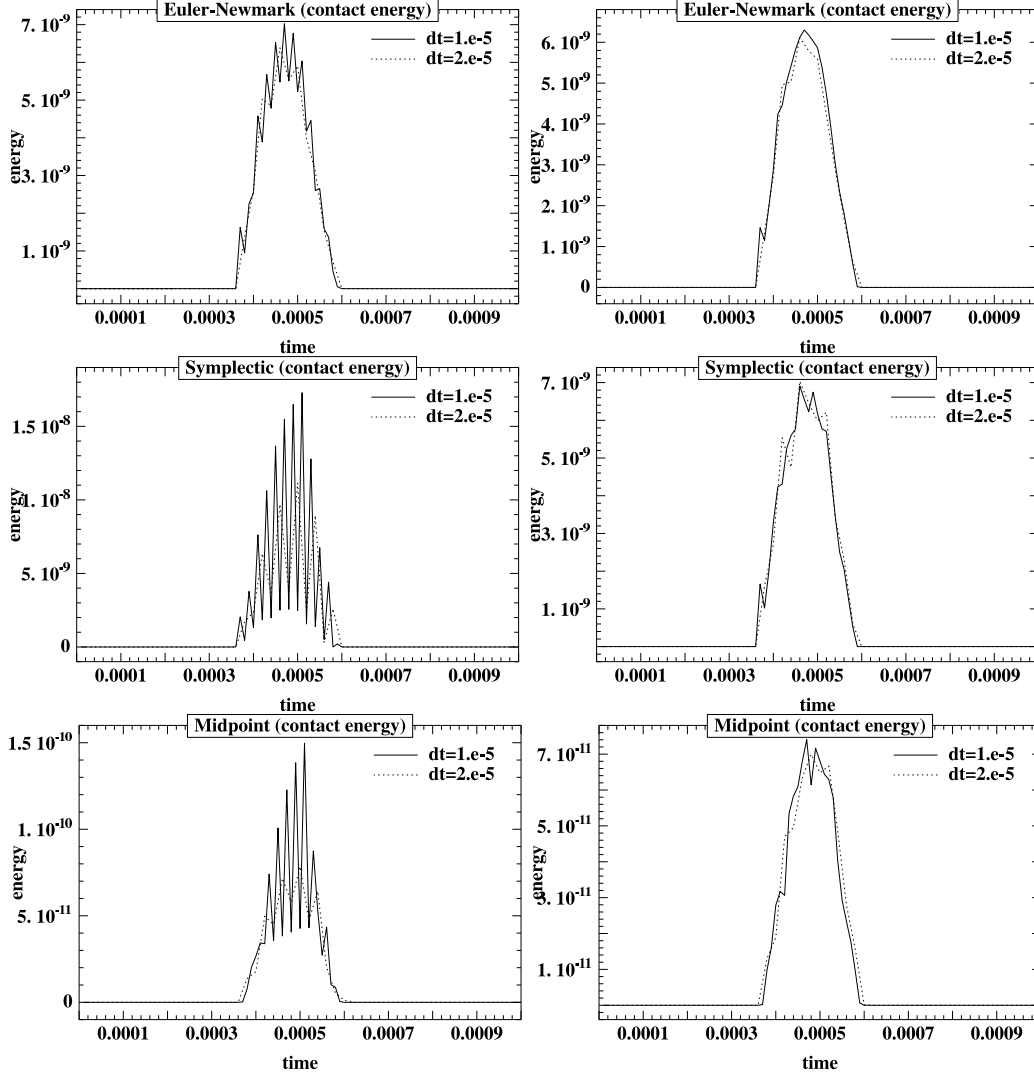


Fig. 8. Contact penalization energy with the standard (left column) and the proposed (right column) approach for the Euler-Newmark, the symplectic scheme from Section 2.4.3, and the symplectic Midpoint scheme using $\Delta t = 5 \cdot 10^{-5} s$ and $\Delta t = 10^{-5} s$ on the sphere.

References

- [1] F. Armero and E. Petöcz. Formulation and analysis of conserving algorithms for frictionless dynamic contact/impact problems. *Comput. Methods Appl. Mech. Engrg.*, 158:269–300, 1998.
- [2] P. Ballard and E. Basseville. Existence and uniqueness for dynamical unilateral contact with coulomb friction: a model problem. *M2AN*, 39(1):59–77, 2005.
- [3] G. Bayada, M. Chambat, K. Lhalouani, and T. Sassi. Éléments finis avec joints pour des problèmes de contact avec frottement de Coulomb non local. *C.R. Acad. Sci. Paris "Analyse numérique"*, 325:1323–1388, 1997.

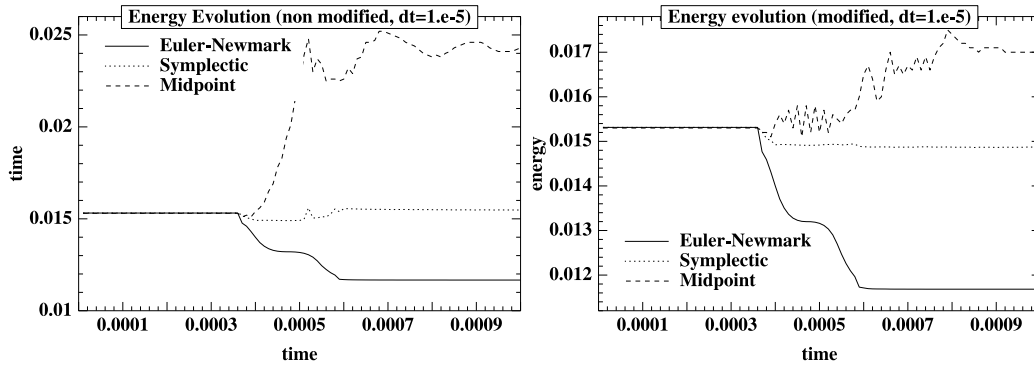


Fig. 9. Comparison of energy evolutions for the frictionless impact of the sphere for the Euler-Newmark, the symplectic scheme from Section 2.4.3, and the symplectic Midpoint scheme, with the proposed modification (left) and the standard approach (right) with time step $\Delta t = 10^{-5} s$.

- [4] F. Ben Belgacem. A stabilized domain decomposition method with non-matching grids for the Stokes problem in three dimensions. *SIAM Journal of Numerical Analysis*, 42(2):667–685, 2004.
- [5] F. Ben Belgacem, P. Hild, and P. Laborde. Approximation of the unilateral contact problem by the mortar finite element method. *C. R. Acad. Sci. Paris Série I. Math.*, 324:123–127, 1997.
- [6] F. Ben Belgacem, P. Hild, and P. Laborde. Extension of the mortar finite element to a variational inequality modeling unilateral contact. *Math. Models Appl. Sci*, 9:287–303, 1999.
- [7] D. Doyen and A. Ern. Convergence of a space semi-discrete modified mass method for the dynamic signorini problem. Preprint 418, CERMICS, 2009.
- [8] G. Duvaut and J-L. Lions. *Les inéquations en Mécanique et en Physique*. Dunod, 1972.
- [9] T.M. Whalen G.C. Archer. Development of rotationally consistent diagonal mass matrices for plate and beam elements. *Comput. Meth. Appl. Mech. Engrg.*, 194(675-689), 2005.
- [10] R.L. Taylor G.L. Goudreau. Evaluation of numerical integration methods in the elastodynamics. *Comput. Meth. Appl. Mech. Engrg.*, 2(69-97), 1972.
- [11] O. Gonzalez. Exact energy and momentum conserving algorithms for general models in nonlinear elasticity. *Comput. Methods Appl. Mech. Engrg.*, 190(13-14):1763–1783, December 2000.
- [12] C. Hager and B. I. Wohlmuth. Analysis of a modified mass lumping method for the stabilization of frictional contact problems. *submitted to Comp. Meth. in Appl. Mech. Engrg.*, 2007.
- [13] E. Hairer, C. Lubich, and G. Wanner. *Geometric Numerical Integration*. Springer-Verlag, 2002.

- [14] P. Hauret. *Numerical methods for the dynamic analysis of two-scale incompressible nonlinear structures*. PhD thesis, Ecole Polytechnique, 2004.
- [15] P. Hauret and P. Le Tallec. Energy-controlling time integration methods for nonlinear elastodynamics, viscoelasticity and impact. *Comp. Meth. App. Mech. Eng.*, (195):4890–4916, 2006.
- [16] P. Hauret and P. Le Tallec. A discontinuous stabilized mortar method for general 3d elastic problems. *Comp. Meth. App. Mech. Eng.*, 196(49):4881–4900, 2007.
- [17] P. Laborde H.B. Khenous and Y. Renard. Comparison of two approaches for the discretization of elastodynamic contact problems. *CRAS Mathématiques*, (342/10):791–796, 2006.
- [18] P. Laborde H.B. Khenous and Y. Renard. On the discretization of contact problems in elastodynamics. *Lecture Notes in Applied Comp. Mech.*, (27):31–38, 2006.
- [19] P. Hild. Numerical implementation of two nonconforming finite element methods for unilateral contact. *Computer Methods in Applied Mechanics and Engineering*, 184(1):99–123, 2000.
- [20] S. Hüeber, A. Matei, and B. Wohlmuth. Efficient algorithms for problems with friction. Technical Report SFB404 #2005-07, Stuttgart University, July 2005.
- [21] S. Hueber and B.I. Wohlmuth. A primal dual active set strategy for nonlinear multibody contact problems. *Comp. Meth. Appl. Mech. Engrg.*, (194):3147–3166, 2005.
- [22] T.J.R. Hughes. Analysis of transient algorithms with particular reference to stability behavior. *Computational Methods for Transient Analysis*, 1(68-155), 1983.
- [23] G.M. Hulbert J. Chung. A family of single -step houbolt time integration algorithms for structural dynamics. *Comput. Meth. Appl. Mech. Engrg.*, 118(1-11), 1994.
- [24] R.H. Gallagher J. Kujawski. A generalized least-squares family of algorithms for transient dynamic analysis. *Earthquake Engineering and Structural Dynamics*, 18(539-550), 1989.
- [25] C. Kane, J.E. Marsden, M. Ortiz, and M. West. Variational integrators and the Newmark algorithm for conservative and dissipative mechanical systems. *International Journal for Numerical Methods in Engineering*, 49:1295–1325, 2000.
- [26] T.A. Laursen. *Computational contact and impact mechanics*. Springer, 2002.
- [27] T.A. Laursen and V. Chawla. Design of energy conserving algorithms for frictionless dynamic contact problems. *International Journal for Numerical Methods in Engineering*, 40:863–886, 1997.

- [28] T.A. Laursen and G.R. Love. Improved implicit integrators for transient impact problems; geometric admissibility within the conserving framework. *Int. J. Num. Meth. Engr.*, 53(2):245–274, January 2002.
- [29] T.A. Laursen and X.N. Meng. A new solution procedure for application of energy-conserving algorithms to general constitutive models in nonlinear elastodynamics. *Computer Methods in Appl. Mech. and Eng.*, 190:6309–6322, September 2001.
- [30] A. Lew, J.-E. Marsden, M. Ortiz, and M. West. Asynchronous variational integrators. *Arch. Ration. Mech. Anal.*, 2003.
- [31] M. Ortiz M. Zielonka and J.E. Marsden. Variational r adaption in elastodynamics. *International Journal for Numerical Methods in Engineering*, 74:1162–1197, 2008.
- [32] J.E. Marsden and M. West. *Acta Numerica*, chapter Discrete mechanics and variational integrators, pages 357–514. Cambridge University Press, 2001.
- [33] J.J. Moreau. Numerical aspects of the sweeping process. *Comput. Methods Appl. Mech. Engrg.*, (177):329–349, 1999.
- [34] R.L. Taylor O.C. Zienkiewicz. *The Finite Element Method Fourth Edition*. McGraw-Hill, 1989.
- [35] M.A. Puso. A 3d mortar method for solid mechanics. *Int. J. Num. Meth. Engr.*, 59:315–336, 2004.
- [36] M.A. Puso and T.A. Laursen. A 3d contact smoothing method using gregory patches. *International Journal for Numerical Methods in Engineering*, 54:1161–1194, 2002.
- [37] P-A Raviart and J-M. Thomas. *Introduction à l'analyse numérique des équations aux dérivées partielles*. Dunod, 1998.
- [38] Y. Renard. A class of well-posed approximations for constrained second order hyperbolic equations. submitted, 2008.
- [39] J.C. Simo and N. Tarnow. The discrete energy-momentum method. conserving algorithms for non linear elastodynamics. *Z angew Math Phys*, 43:757–792, 1992.
- [40] W.L. Mindle T. Belytschko. Flexural wave propagation behavior of lumped mass approximations. *Computers and Structures*, 12(805-812), 1980.
- [41] P. Le Tallec, F. Dambakizi, and P. Hauret. Numerical solution of dynamic contact problems. In N.D. Lagaros M. Papadrakakis, D.C. Charmpis and Y. Tsompanakis, editors, *ECCOMAS Thematic Conference of Computational Methods in Structural Dynamics and Earthquake Engineering*, Rethymno, Crete, Greece, June 2007.
- [42] P. Le Tallec and S. Mani. Numeric analysis of a linearized fluid-structure interaction problem. *Numerische Mathematik*, 87:317–354, 2000.

- [43] B.I. Wohlmuth. A mortar finite element method using dual spaces for the Lagrange multiplier. *SIAM J. Numer. Anal.*, 38:989–1012, 2000.
- [44] Barboteu Y. Ayyad, M and R. Fernandez. A frictionless viscoelastodynamic contact problem with energy consistent properties: numerical analysis and computational aspects. *Comput. Meth. Appl. Mech. Engrg.*, 198(669-679), 2009.