ENERGY CONSERVING ALGORITHMS FOR A CO-ROTATIONAL FORMULATION

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Abstract. Linearizations of the Saint Venant–Kirchoff model for elastic bodies are often considered in numerical simulations. A linearization of the elastic terms with respect to the displacement does not provide satisfying numerical results when considering large global motions (even with small deformations). In order to tackle this problem, we propose time discretized conservative algorithms that uses a specific linearization derived from the co-rotational formulation. The motion of the body is decomposed into global translation and rotation and a local displacement. Our new algorithms result in a coupled nonlinear system in which the local displacements enter linearly. Existence of a solution for the fully discrete setting which preserves the energy and the angular momentum is established. Numerical results illustrate the flexibility and efficiency of the proposed algorithms.

Key words. Elastodynamic, co-rotational formulation, energy conservative schemes, large displacements, small strains.

AMS subject classifications. 35L70, 74B05, 74B20, 74H15.

1. Introduction. The simulation of elastodynamic problems involving large rotation and translation is a well-known challenge in modeling of continuum mechanic problems, e.g., in the aerospace industry. A correct definition of a global angle of rotation for an elastic body is not straightforward and requires costly computations. Especially the treatment of high-speed rotations is a significant issue in finite element discretization and the development of suitable time-integration schemes.

Usually, geometrical nonlinear material laws are applied to tackle these kind of problems. In contrast to the linear elasticity setting, the rigid body motions, i.e., rotations and translations, do not contribute to the elastic energy. However, the resulting equations cannot be solved directly, but a more expensive iteration scheme has to be applied. Moreover, when considering high-speed rotation with large timesteps, this method shows unsatisfying numerical results, more precisely, in those cases the approximation of the rotation is quite bad and spurious oscillation might be observed.

A first way to tackle these problem consists in linearizing the evolution equation with respect to parameters associated to the displacement of the body, i.e., to work in the linear elasticity framework. Linearization with respect to the displacement itself does not shows satisfying results, though other approaches have given good results, see, e.g., [32].

A promising approach is to split the motion into a rigid body motion (translation and rotation) and a purely elastic deformation. The main advantage of this method is to reduce the magnitude of the displacement under consideration. Initially introduced in [10] to tackle problems involved in the aircraft and spacecraft dynamics, the motivation was essentially to trace the global motion of a given body. This approach was put in an abstract framework by Fraeijis de Veubeke [19], where different criteria are presented to guarantee the uniqueness of the decomposition. Nowadays, this idea is often used by the engineering community where it is referred as “co-rotational formulation”.

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Let us draw in more detail some developments of this approach. The problem of handling large rotations in the Lagrangian kinematic descriptions of continuum mechanics has spawned several publications, e.g., [1, 2, 3, 22]. The application of the splitting of the deformation in combination with finite elements was introduced by Wempner [34] and Belytschko and Hsieh [7]. In the engineering literature, the term “co-rotational finite elements” was established for this method starting with [5, 6] where the splitting is used for each element, resulting in additional degrees of freedom per element. Some developments of this approach have been presented in [16, 17, 31, 33]. The method was improved by defining a co-rotated frame per element [8, 9], see also the overview [24]. Crisfield [12, 13] developed the concept of consistent linearization in the co-rotational formulation. Rankin and Brogan finally invented the element independent co-rotational formulation, [23, 29, 30], where projectors are used to separate the total deformation. Recently, the co-rotational formulation has been used for control and regulation [4, 25], sensitivity analysis [26, 27, 28] and modern solving techniques for real-life simulations [14, 15]. For a more exhaustive overview over the development of the co-rotational formulation, we refer to [18].

However, the design of suitable time integration methods for the co-rotational framework is still an open question, see topic E of Section 7 in [18]. In particular, time-discretized schemes often preserve the total energy of the body only asymptotically, preventing for using large timesteps. To fill this gap, we present in this paper energy conserving time discretizations associated to a co-rotational formulation. The equation under consideration is obtained through a linearization with respect to the displacement obtained after having decomposed the motion into a global rigid body motion and local (small) deformation. We use Fraeijis de Veubeke’s criterion and choose the co-rotational decomposition that minimizes the L^2 -norm of this displacement. The well-posedness of the resulting system has been proved recently in [20, 21]. In this way, the linearization remains a very efficient approach to accelerate the computation while obtaining a correct approximation of the motion, as we show in various examples. In addition, we note that the results on the time integration schemes can be directly applied to the original system and that the efficiency of the numerical simulation is not restricted to situations with small local deformations.

Though most of the concepts presented in this paper holds both for $2D$ and $3D$, we focus in our presentation on the $2D$ -case for reason of simplicity. The necessary adaptations to $3D$ are however also presented together with a $3D$ version of one of our algorithm.

The rest of the paper is organized as follows: In Section 2, we derive the $2D$ model and present the continuous linearized system of equations describing the evolution of the system. We give two time-discretized energy conservative algorithms in Section 3. We discuss in Section 4 the space discretization on a constrained space and the existence of a solution. In Section 5, we extend one of our algorithm to the $3D$ -case. Finally, in Section 6, we show the efficiency and flexibility of our approach through various numerical tests.

2. Model. Throughout this paper, we use the notation:

$$\dot{a}(x, t) := \frac{\partial}{\partial t} a(x, t), \quad \ddot{a}(x, t) := \frac{\partial^2}{\partial t^2} a(x, t).$$

Given a matrix A , we denote by $A^\top$ its transposed matrix and by $tr(A)$ its trace. The identity matrix of $\mathbb{R}^2$ is denoted by I , R_θ represents the rotation of θ , $\Pi := R_{\frac{\pi}{2}}$

FIG. 2.1. Calculated rotation speed using standard time discretization. Left: Rigid body motion, Right: rotation plus oscillation

and $A : B := \text{tr}(A^\top B)$ is the usual matrix scalar product. We note that using this notation the derivative of the rotation matrix reads $\frac{d}{d\theta} R_\theta = \Pi R_\theta$.

2.1. Nonlinear model. Let $\Omega \subset \mathbb{R}^2$ be a bounded domain with a piecewise sufficiently smooth boundary $\Gamma := \partial\Omega$ describing an elastic body considered to be a Saint Venant–Kirchhoff material of mass density $\rho(x)$. The coordinate system is chosen such that the center of gravity has the coordinates $(0, 0)$, i.e., $\int_\Omega \rho x = 0$. The body is subject to some volume forces $f(x, t)$ and boundary tractions $g(x, t)$. Let $\varphi : \Omega \times [0, T] \rightarrow \mathbb{R}^2$ be the deformation mapping. In the fully nonlinear setting, the evolution of φ is described by the weak form of the following equilibrium condition [11]:

$$\int_\Omega \rho \dot{\varphi} \cdot \eta + \int_\Omega \frac{\partial}{\partial F} W(E(\varphi - x)) : \nabla \eta = \int_\Omega f \cdot \eta + \int_\Gamma g \cdot \eta, \quad (2.1)$$

where η is a function in $V := [H^1(\Omega)]^2$ and $F := \nabla(\varphi - x)$ the deformation gradient. For a given displacement d , the stored energy $W(E(d))$ is:

$$W(E(d)) := \frac{\lambda}{2} (\text{tr}(E(d)))^2 + \mu \text{tr}(E(d)^2),$$

where λ and μ are the Lamé parameters and

$$E(d) := \frac{1}{2} (\nabla d + \nabla d^\top + \nabla d^\top \nabla d). \quad (2.2)$$

Energy- and momentum-conserving time-integration schemes for this setting are well-known, see, e.g., [32]. However, when considering high-speed rotation or large time-steps, these standard time integration schemes show poor accuracy: In this case, the rotation speed is not reproduced correctly resulting in a wrong solution. In Figure 2.1, we show two examples demonstrating this and refer to Section 6 for details. The first example is a rigid body motion with a constant rotation speed of 20, see Example 1 in the numerical part. In the second example (Example 3), a rigid body motion with high-speed elastic oscillations is depicted. These high-speed oscillations cannot be resolved for large timesteps. Yet, it turns out that the standard time integration schemes not only reproduce a wrong mean value of the rotational speed but also artificially increase the oscillation.

2.2. Co-rotational decomposition of the motion. As a remedy, the co-rotational formulation proposes to work with displacements in smaller spaces, by removing the possible large rigid body motions of the displacement involved in the elastic term of (2.1). The deformation is decomposed as follows [21]:

$$\varphi(x, t) = \tau(t) + R_{\theta(t)}(x + u(x, t)). \quad (2.3)$$

In this equation, $\tau(t) \in \mathbb{R}^2$ describes the global translation of the body and R_θ its global rotation. After this change of variable, the displacement is described by u . An important property of the decomposition (2.3) is that:

$$E(\varphi - x) = E(u), \quad (2.4)$$

which shows that the nonlinear model correctly cancels the global translation and rotation appearing in φ . In order to define a unique triplet (τ, θ, u) and to work with small displacements, we consider the decomposition that minimizes the weighted L^2 -norm of u , $\int_\Omega \rho |u|^2$, see [19]. A straightforward computation shows that if $\int_\Omega \rho(x + u) \cdot x \neq 0$, this minimization condition for u is equivalent to (see [20, 21]):

$$\int_\Omega \rho u = 0, \quad \int_\Omega \rho u \cdot \Pi x = 0. \quad (2.5)$$

We note that the first condition results from the translation and the second condition from the rotation term. Thus, we are looking for the displacement u in the linear space $X := X^{\text{trans}} \cap X^{\text{rot}}$ defined by:

$$X^{\text{trans}} := \left\{ u \in V; \int_\Omega \rho u = 0 \right\}, \quad X^{\text{rot}} := \left\{ u \in V; \int_\Omega \rho u \cdot \Pi x = 0 \right\}.$$

Let us now consider the effects of this change of variable on Equation (2.1).

We start with the elastic term of (2.1). Defining $\hat{F} := \nabla u$, we have, thanks to (2.4):

$$\begin{aligned} \int_\Omega \frac{\partial}{\partial F} W(E(\varphi - x)) : \nabla \eta &= \int_\Omega R_\theta \frac{\partial}{\partial \hat{F}} W(E(\varphi - x)) : \nabla \eta \\ &= \int_\Omega R_\theta \Sigma(u) : \nabla \eta, \end{aligned}$$

where $\Sigma(u) := \frac{\partial}{\partial \hat{F}} W(E(u))$.

The inertial term of (2.1) can also be rewritten in this new setting. In what follows, we will make a great use of the relative velocity that will simplify our presentation. We define it by:

$$s(x, t) := R_{\theta(t)}^\top (\dot{\varphi}(x, t) - \dot{\tau}(t)) = \dot{u}(x, t) + \dot{\theta}(t) \Pi(x + u(x, t)). \quad (2.6)$$

The acceleration term can then be expressed by

$$\ddot{\varphi}(x, t) = \ddot{\tau}(t) + R_{\theta(t)} \left(\dot{s}(x, t) + \dot{\theta}(t) \Pi s(x, t) \right). \quad (2.7)$$

Using this representation of $\ddot{\varphi}$ and reducing the testspace to X , (2.1) now reads

$$\int_\Omega \rho \left(\dot{s} + \dot{\theta} \Pi s \right) \cdot v + \int_\Omega \Sigma(u) : \varepsilon(v) = F_\theta(v), \quad \forall v \in X, \quad (2.8)$$

where we have set $v = R_\theta^\top \eta$ and

$$F_\theta(v) := \int_\Omega f \cdot R_\theta v + \int_\Gamma g \cdot R_\theta v.$$

We note that the term $\ddot{\tau} \cdot R_\theta v$ cancels because $R_\theta v \in X^{\text{trans}}$. To compensate this reduction of the testspace, additional constraints have to be imposed. These ones

are then used to determine the correct values of θ and τ . Thus, in addition to (2.8), we require that the linear and angular momentum are preserved. To obtain the corresponding equation, we formally test (2.8) with $v_{\text{trans}} = R_\theta^\top(0, 1)^\top$, $v_{\text{trans}} = R_\theta^\top(1, 0)^\top$ and $v_{\text{rot}} = \Pi(x + u)$, respectively, to get the linear and angular momentum equations. Using $u \in X^{\text{trans}}$, this gives the conservation of the linear momentum,

$$\mathcal{M}\ddot{\tau} = \int_{\Omega} f + \int_{\Gamma} g, \quad (2.9)$$

and the conservation of the angular momentum,

$$\dot{\mathcal{J}} = F_\theta(\Pi(x + u)), \quad (2.10)$$

where $\mathcal{M}$ and $\mathcal{J}$ are defined by

$$\mathcal{M} := \int_{\Omega} \rho, \quad \mathcal{J} := \int_{\Omega} \rho s \cdot \Pi(x + u).$$

2.3. Linearization. In order to accelerate the computation or when considering numerical methods to solve (2.8), some linearizations can be done. In this paper, we focus on algorithms concerning the model obtained by linearizing the elastic term of (2.8). This is done by the following approximation of (2.2):

$$E(u) \approx \varepsilon(u) := \frac{1}{2}(\nabla u + \nabla u^\top),$$

which leads to

$$\int_{\Omega} \rho \left(\dot{s} + \dot{\theta} \Pi s \right) \cdot v + \int_{\Omega} \sigma(u) : \varepsilon(v) = F_\theta(v). \quad (2.11)$$

where $\sigma(u) := 2\mu\varepsilon(u) + \lambda \text{tr} \varepsilon(u)I$. We will consider the nonlinear model (2.8) as a reference to evaluate the efficiency of our algorithms.

Let us now introduce the space Y , defined by:

$$Y := \left\{ u \in X; \int_{\Omega} \rho(x + u) \cdot x > 0 \right\}.$$

In a recent paper [20] (see also [21]), Grandmont *et al.* have obtained the following existence result concerning the system (2.9)–(2.10)–(2.11):

THEOREM 2.1. *Let $\tau_0, \dot{\tau}_0$ be given in $\mathbb{R}^2$, $\theta_0, \dot{\theta}_0$ be real numbers, $u_0 \in Y$, $\dot{u}_0 \in L^2(\Omega)$, $f \in L^2_{\text{loc}}(0, +\infty; L^2(\Omega))$ and $g \in H^1_{\text{loc}}(0, +\infty; H^{-\frac{1}{2}}(\Gamma) \cap L^2_{\text{loc}}(0, +\infty; L^1(\Gamma)))$. There exists $T^* > 0$ such that for all $T < T^*$ there exists a unique triplet (τ, θ, u) with $\tau \in H^2(0, T)$, $\theta \in H^2(0, T)$, $u \in H^2(0, T; (H^1(\Omega))' \cap W^{1,\infty}(0, T; L^2(\Omega))) \cap L^\infty(0, T; H^1(\Omega))$ and $u \in \mathcal{C}^0([0, T]; Y)$ satisfying*

$$\begin{cases} \mathcal{M}\ddot{\tau} = \int_{\Omega} f + \int_{\Gamma} g \text{ in } L^2(0, T) \\ \dot{\mathcal{J}} = F_\theta(\Pi(x + u)) \text{ in } \mathcal{D}'(0, T) \\ \forall v \in X, \int_{\Omega} \rho \left(\dot{s} + \dot{\theta} \Pi s \right) \cdot v + \sigma(u) : \varepsilon(v) = F_\theta(v) \text{ in } \mathcal{D}'(0, T) \end{cases} \quad (2.12)$$

where s is defined by (2.6) together with $\tau(0) = \tau_0$, $\dot{\tau}(0) = \dot{\tau}_0$, $\theta(0) = \theta_0$, $\dot{\theta}(0) = \dot{\theta}_0$, $u(0) = u_0$, $\dot{u}(0) = \dot{u}_0$.

Moreover, the following alternative holds:

- $T^* = +\infty$ or
- $\lim_{t \rightarrow T^*} \int_{\Omega} \rho(x + u) \cdot x = 0$.

3. Energy conservative algorithms. We now present our energy conservative algorithms which are based on two different time discretizations of (2.12). The first one guarantees the conservation of the energy, but not of the angular momentum. In addition, an alternative scheme preserving the energy and the angular momentum is presented. To start we briefly outline the strategies we have followed to design our algorithms. Denoting by $\frac{d}{dt}$ the time derivation operator, we find in terms of (2.6) and (2.7):

$$R_\theta^\top (\ddot{\varphi} - \ddot{\tau}) = \left(\frac{d}{dt} + \dot{\theta}\Pi \right) s, \quad (3.1)$$

$$\begin{aligned} &= \left(\frac{d}{dt} + \dot{\theta}\Pi \right)^2 (x + u) \\ &= \ddot{u} + \Pi \left(\frac{d}{dt}(\dot{\theta}u) + \dot{\theta}\dot{u} \right) - (\dot{\theta})^2(x + u). \end{aligned} \quad (3.2)$$

The first algorithm is obtained by discretizing each term of (3.2). In the second algorithm, we first discretize $s = (\frac{d}{dt} + \dot{\theta}\Pi)(x + u)$, see (3.14), and then discretize $R_\theta^\top (\ddot{\varphi} - \ddot{\tau})$ via (3.1), see the first term of (3.13).

3.1. Mid-point time discretization and discrete setting. Let us denote by n the time index. We use a mid-point time discretization which has the property:

$$\dot{a}_{n+1/2}b_{n+1/2} + a_{n+1/2}\dot{b}_{n+1/2} = [ab]_{n+1/2}, \quad (3.3)$$

where we have used the following notations:

$$\star_{n+1/2} := \frac{\star_{n+1} + \star_n}{2}, \quad \dot{\star}_{n+1/2} := \frac{\star_{n+1} - \star_n}{\Delta t}, \quad (3.4)$$

with Δt the timestep and $\star$ a generic time-discretized quantity.

Let us also define the total energy of the linearized system at the timestep n by

$$\mathcal{E}_n := \frac{1}{2}\mathcal{M}\dot{\tau}_n^2 + \frac{1}{2}\int_{\Omega}\rho s_n^2 + \frac{1}{2}\int_{\Omega}\sigma(u_n) : \varepsilon(u_n), \quad (3.5)$$

The angular momentum is defined by

$$\mathcal{J}_n := \int_{\Omega}\rho s_n \cdot \Pi(x + u_n). \quad (3.6)$$

Here s_n is a time discretization of (2.6), depending on the algorithm under consideration.

Note that the full nonlinear energy is defined by:

$$\mathcal{E}_n^{nl} := \frac{1}{2}\mathcal{M}\dot{\tau}_n^2 + \frac{1}{2}\int_{\Omega}\rho s_n^2 + \frac{1}{2}\int_{\Omega}\Sigma(u_n) : \varepsilon(u_n),$$

which coincides with (3.5) when neglecting terms of second order with respect to ∇u .

Finally, we discretize F_θ at the timestep $(n + 1/2)$ by:

$$F_{n+1/2}(v) := \int_{\Omega} f_{n+1/2} \cdot R_{\theta_{n+1/2}} v + \int_{\Gamma} g_{n+1/2} \cdot R_{\theta_{n+1/2}} v.$$

3.2. Algorithm I. A time discretization of (2.12) can be done in terms of (3.2). Special care has to be taken about the energy-conservation property. To this end, we choose some special approximations such as $\left(\dot{\theta}(t_{n+1/2})\right)^2 \approx \dot{\theta}_n \dot{\theta}_{n+1}$.

Algorithm I then reads: Given $\tau_0, \dot{\tau}_0, \theta_0, \dot{\theta}_0, u_0$, the external forces $(f_{n+1/2})_{n \in \mathbb{N}}$ and $(g_{n+1/2})_{n \in \mathbb{N}}$, and suppose that $\tau_n, \dot{\tau}_n, \theta_n, \dot{\theta}_n$ and $u_n, \dot{u}_n \in X$ have already been computed. The derivation of $\tau_{n+1}, \dot{\tau}_{n+1}, \theta_{n+1}, \dot{\theta}_{n+1}$ and $u_{n+1}, \dot{u}_{n+1} \in X$ is carried out by solving:

$$\mathcal{M}\ddot{\tau}_{n+1/2} = \int_{\Omega} f_{n+1/2} + \int_{\Gamma} g_{n+1/2}, \quad (3.7)$$

$$\begin{aligned} \frac{1}{\Delta t} \left(\int_{\Omega} \rho \dot{\theta}_{n+1} (x + u_{n+1})^2 - \int_{\Omega} \rho \dot{\theta}_n (x + u_n)^2 \right) + \int_{\Omega} \rho \Pi \frac{\dot{\theta}_{n+1} u_{n+1} + \dot{\theta}_n u_n}{2 \dot{\theta}_{n+1/2}} \cdot \ddot{u}_{n+1/2} \\ = F_{n+1/2}(\Pi(x + u_{n+1/2})), \end{aligned} \quad (3.8)$$

$$\begin{aligned} \int_{\Omega} \rho \left(\ddot{u}_{n+1/2} + \Pi \frac{\dot{\theta}_{n+1} u_{n+1} - \dot{\theta}_n u_n}{\Delta t} + \Pi \dot{\theta}_{n+1/2} \dot{u}_{n+1/2} - \dot{\theta}_n \dot{\theta}_{n+1} (x + u_{n+1/2}) \right) \cdot v \\ + \int_{\Omega} \sigma(u_{n+1/2}) : \varepsilon(v) = F_{n+1/2}(v) \quad \forall v \in X. \end{aligned} \quad (3.9)$$

Equations (3.7) – (3.9) correspond to the three equations of (2.12). We refer to Section 4 for details about how to guarantee that $u_{n+1} \in X$.

We note that using the discretized relative velocity

$$s_n := \dot{u}_n + \dot{\theta}_n \Pi(x + u_n), \quad (3.10)$$

and the fact that $u_n, \dot{u}_n \in X$, the angular momentum $\mathcal{J}_n$ can be written as

$$\mathcal{J}_n = \int_{\Omega} \rho s_n \cdot \Pi(x + u_n) = \dot{\theta}_n \int_{\Omega} \rho (x + u_n)^2 + \int_{\Omega} \rho \dot{u}_n \cdot \Pi u_n.$$

This quantity is not preserved exactly by Algorithm I, because of the third term of the left hand side of (3.8). It is however possible to specify the local order with respect to Δt . Indeed, we have:

$$\mathcal{J}_{n+1} - \mathcal{J}_n - \Delta t F_{n+1/2}(\Pi(x + u_{n+1/2})) = \frac{\Delta t^2}{4} \frac{\ddot{\theta}_{n+1/2}}{\dot{\theta}_{n+1/2}} \Pi \dot{u}_{n+1/2} \cdot \ddot{u}_{n+1/2},$$

Although the momentum is asymptotically preserved if Δt tends to zero, we observe that local oscillations occur, see Figure 3.1. This motivates the introduction of Algorithm II.

3.3. Algorithm II. Let us now describe a time discretization of (2.12) that preserves both the energy and the angular momentum.

Given $\tau_0, \dot{\tau}_0, \theta_0, u_0, s_0$, the external forces $(f_{n+1/2})_{n \in \mathbb{N}}$ and $(g_{n+1/2})_{n \in \mathbb{N}}$, and suppose that $\tau_n, \dot{\tau}_n, \theta_n, u_n \in X$ and s_n have already been computed. The derivation of $\tau_{n+1}, \dot{\tau}_{n+1}, \theta_{n+1}, u_{n+1} \in X$ and $s_{n+1} \in V$ is carried out by solving:

$$\mathcal{M}\ddot{\tau}_{n+1/2} = \int_{\Omega} f_{n+1/2} + \int_{\Gamma} g_{n+1/2}, \quad (3.11)$$

$$\dot{\mathcal{J}}_{n+1/2} = F_{n+1/2}(\Pi(x + u_{n+1/2})), \quad (3.12)$$

$$G(\dot{s}_{n+1/2}, s_{n+1/2}, \dot{\theta}_{n+1/2}, u_{n+1/2}; v) = F_{n+1/2}(v) \quad \forall v \in X, \quad (3.13)$$

FIG. 3.1. Angular momentum using Algorithm I and II.

with

$$G(\dot{s}, s, \dot{\theta}, u; v) := \int_{\Omega} \rho(\dot{s} + \dot{\theta}\Pi s) \cdot v + \int_{\Omega} \sigma(u) : \varepsilon(v)$$

and

$$s_{n+1/2} := \dot{u}_{n+1/2} + \dot{\theta}_{n+1/2}\Pi(x + u_{n+1/2}). \quad (3.14)$$

Equations (3.11) – (3.13) correspond to the three equations of (2.12). Equation (3.12) guarantees that the angular momentum is preserved by this algorithm.

Remark: We note that the time discretization of the auxiliary variable s is done at the timestep n , see (3.10), in Algorithm I and at the staggered timestep $(n + 1/2)$, see (3.14), in Algorithm II. Moreover, given a parameter $\star$ and denoting by $\star^I$ and $\star^{II}$ its time discretizations in Algorithm I and Algorithm II respectively, we have that:

$$s_{n+1/2}^I = s_{n+1/2}^{II} + \frac{\Delta t^2}{4} \dot{\theta}_{n+1/2} \Pi \dot{u}_{n+1/2}^{II}.$$

3.4. Energy conservation. Let us state the main property of our algorithms.

THEOREM 3.1. *Algorithms I and II defined by (3.7)–(3.9) and (3.11)–(3.13), respectively, guarantee the energy conservation in the sense that:*

$$\mathcal{E}_{n+1} - \mathcal{E}_n = \Delta t \left(\int_{\Omega} f_{n+1/2} \cdot \dot{\varphi}_{n+1/2} + \int_{\Gamma} g_{n+1/2} \cdot \dot{\varphi}_{n+1/2} \right).$$

Here, $\mathcal{E}$ is the total energy defined by (3.5) where s is defined by (3.10) when considering Algorithm I and by (3.14) when considering Algorithm II. The time discretization of $\dot{\varphi}$ is done by:

$$\dot{\varphi}_{n+1/2} := \dot{\tau}_{n+1/2} + R_{\theta_{n+1/2}} s_{n+1/2}.$$

Proof. We only give the proof for the case of Algorithm II, since the one corresponding to Algorithm I can be obtained in a similar way.

Testing (3.13) with $v = \dot{u}_{n+1/2}$, we find:

$$\int_{\Omega} \rho(\dot{s}_{n+1/2} + \dot{\theta}_{n+1/2}\Pi s_{n+1/2}) \cdot \dot{u}_{n+1/2} + \int_{\Omega} \sigma(u_{n+1/2}) : \varepsilon(\dot{u}_{n+1/2}) = F_{n+1/2}(\dot{u}_{n+1/2}). \quad (3.15)$$

On the other hand, using (3.3), (3.12) reads:

$$\int_{\Omega} \rho \dot{s}_{n+1/2} \cdot \Pi(x + u_{n+1/2}) + \int_{\Omega} \rho s_{n+1/2} \cdot \Pi \dot{u}_{n+1/2} = F_{n+1/2}(\Pi(x + u_{n+1/2})). \quad (3.16)$$

Then, multiplying (3.16) by $\Delta t \dot{\theta}_{n+1/2}$, (3.15) by Δt and adding the two resulting equations, we get by means of (3.14):

$$\begin{aligned} \Delta t \int_{\Omega} \rho \dot{s}_{n+1/2} \cdot (\dot{u}_{n+1/2} + \dot{\theta}_{n+1/2} \Pi(x + u_{n+1/2})) + \Delta t \int_{\Omega} \sigma(u_{n+1/2}) : \varepsilon(\dot{u}_{n+1/2}) \\ = \frac{1}{2} \left(\int_{\Omega} \rho s_{n+1}^2 + \sigma(u_{n+1}) : \varepsilon(u_{n+1}) - \int_{\Omega} \rho s_n^2 + \sigma(u_n) : \varepsilon(u_n) \right), \end{aligned}$$

and thus:

$$\frac{1}{2} \left(\int_{\Omega} \rho s_{n+1}^2 + \sigma(u_{n+1}) : \varepsilon(u_{n+1}) - \int_{\Omega} \rho s_n^2 + \sigma(u_n) : \varepsilon(u_n) \right) = \Delta t F_{n+1/2}(s_{n+1/2}). \quad (3.17)$$

Finally, using (3.11), we find:

$$\frac{1}{2} \mathcal{M} \dot{\tau}_{n+1}^2 - \frac{1}{2} \mathcal{M} \dot{\tau}_n^2 = \Delta t \left(\int_{\Omega} f_{n+1/2} \cdot \dot{\tau}_{n+1/2} + \int_{\Gamma} g_{n+1/2} \cdot \dot{\tau}_{n+1/2} \right),$$

which yields in combination with (3.17) the energy conservation. $\square$

Concluding, we remark that only Algorithm II yields both energy and angular momentum conservation. In Figure 3.1, the angular momentum for the two different algorithms is compared. The problem setting and parameters of this example are given in Section 6.2.

4. Space discretization. In this section, we present a suitable space discretization for the time-discretized systems. We focus on (3.13) although the same method can be used for the discretization of (3.9). The space X motivates the use of a Galerkin method based on the spectral decomposition of the operator $-\operatorname{div}(\sigma(\cdot))$. Indeed, we note that X is spanned by the eigenvectors with non-zero eigenvalue and is orthogonal (in the sense of the $L^2(\Omega)$ scalar product) on the kernel of this operator.

Unfortunately, finite elements do not fit into this setting. We observe that (2.5) is not satisfied by nodal finite element basis functions. The orthogonal projection of this basis functions onto the space X leads to a non-local support of the finite element basis and additional computational costs. We therefore use a Lagrange multiplier approach to guarantee these conditions and state the problem in a saddle point framework. For this fully discretized algorithm, we show existence of a solution of (3.11)–(3.13).

4.1. Finite element approximation of the space X . We assume that the domain Ω is resolved by a mesh consisting of quadrilaterals and/or triangles. We use a conforming finite element space of lowest order and denote the nodal basis functions by ϕ_i and the finite element space by V_h . The mass matrix is denoted by M , $M_{ij} := \int_{\Omega} \rho \phi_i \cdot \phi_j$, and the stiffness matrix for the linearized material law by S , $S_{ij} := \int_{\Omega} \sigma(\phi_i) : \varepsilon(\phi_j)$. The subspace X_h of X is defined by $X_h := X \cap V_h$.

To guarantee that $u \in V_h$ is also in X_h , i.e., satisfies (2.5), we introduce two

Lagrange multipliers $\alpha \in \mathbb{R}$ and $\beta \in \mathbb{R}^2$. Then, (3.13) can be rewritten as

$$\begin{aligned} G(\dot{s}_{n+1/2}, s_{n+1/2}, \dot{\theta}_{n+1/2}, u_{n+1/2}; v) + \alpha \int_{\Omega} \rho v \cdot \Pi x + \int_{\Omega} \rho \beta \cdot v &= F_{n+1/2}(v), \quad \forall v \in V_h \\ \int_{\Omega} \rho u_{n+1/2} \cdot \Pi x &= 0, \\ \int_{\Omega} \rho u_{n+1/2} &= 0. \end{aligned} \quad (4.1)$$

The Lagrange multiplier β can be easily eliminated by static condensation. First, we recall that $s_n, u_n, u_{n+1/2} \in X^{\text{trans}}$. This implies $\int_{\Omega} \rho \Pi u_{n+1/2} = \Pi \int_{\Omega} \rho u_{n+1/2} = 0$; therefore $\Pi u_{n+1/2} \in X^{\text{trans}}$ and thus $s_{n+1/2}, \dot{s}_{n+1/2} \in X^{\text{trans}}$. Using a constant $v \in V_h$, we see that $\varepsilon(v) = 0$ and therefore $G(\dot{s}_{n+1/2}, s_{n+1/2}, \dot{\theta}_{n+1/2}, u_{n+1/2}; v) = 0$. We use $v = (1, 0)^{\top}$ and $v = (0, 1)^{\top}$, respectively, in (4.1) and finally obtain

$$\beta = \frac{1}{\mathcal{M}} \left(\int_{\Omega} R_{\theta_{n+1/2}}^{\top} f_{n+1/2} + \int_{\Gamma} R_{\theta_{n+1/2}}^{\top} g_{n+1/2} \right) = R_{\theta_{n+1/2}}^{\top} \ddot{\tau}_{n+1/2}. \quad (4.2)$$

Using (4.2) in (4.1) gives the following system:

$$\begin{aligned} G(\dot{s}_{n+1/2}, s_{n+1/2}, \dot{\theta}_{n+1/2}, u_{n+1/2}; v) + \alpha \int_{\Omega} \rho v \cdot \Pi x &= \tilde{F}_{n+1/2}(v) \quad \forall v \in V_h, \\ \int_{\Omega} \rho u_{n+1/2} \cdot \Pi x &= 0, \end{aligned} \quad (4.3)$$

where $\tilde{F}_{n+1/2}$ is defined by

$$\tilde{F}_{n+1/2}(v) := F_{n+1/2}(v) - \int_{\Omega} \rho R_{\theta_{n+1/2}}^{\top} \ddot{\tau}_{n+1/2} \cdot v.$$

We note that the first line of (4.3) ensures $\int_{\Omega} \rho u_{n+1/2} = 0$, i.e., $u_{n+1/2} \in X^{\text{trans}}$.

We rewrite the system in terms of $u_{n+1/2}$ and obtain the following linear system for the coefficients vector.

$$\left(\begin{array}{c|c} \tilde{G}(\theta_{n+1} - \theta_n, \Delta t) & M \Pi x \\ \hline (M \Pi x)^{\top} & 0 \end{array} \right) \cdot \left(\begin{array}{c} u_{n+1/2} \\ \hline \alpha_{n+1/2} \end{array} \right) = \left(\begin{array}{c} \tilde{c}_{n+1/2}(\theta_{n+1} - \theta_n, \Delta t) \\ \hline 0 \end{array} \right), \quad (4.4)$$

where:

- $\tilde{G}(\delta, \Delta t) := M(2I + \delta \Pi)^2 + \Delta t^2 S$,
- $\tilde{c}_{n+1/2}(\delta, \Delta t) := M(2I + \delta \Pi)(2u_n - \delta \Pi x) + 2M \Delta t s_n + \Delta t^2 \tilde{F}_{n+1/2}$.

We note that we use the widely applied abuse of notation, i.e., the symbols $u_n, u_{n+1/2}, s_n$ and $\tilde{F}_{n+1/2}$ are used depending on the situation as the function or the coefficient vector of the finite element representation. We also keep the notation "·" for the scalar product in what follows.

Equation (3.12) now reads

$$h(\theta_{n+1} - \theta_n, \Delta t) = 0 \quad (4.5)$$

with:

$$h(\delta, \Delta t) := 4\delta(x + u_{n+1/2}) \cdot M(x + u_{n+1/2}) \\ + \left(-\delta M(x + u_n) + 2\Delta t M \Pi s_n + \Delta t^2 \Pi R_{\theta_n + \delta/2}^\top \tilde{F}_{n+1/2} \right) \cdot (x + u_{n+1/2}),$$

where $u_{n+1/2}$ is the solution of (4.4) corresponding to $\theta_{n+1} - \theta_n = \delta$.

4.2. Existence of a solution for the fully discretized algorithm. This section is devoted to the existence of a solution of the fully discretized system associated with Algorithm II.

THEOREM 4.1. *Given $\mathcal{E}_{max} > 0$, $F_{max} > 0$ and $\nu > 0$, suppose that at the step n , $\mathcal{E}_n \leq \mathcal{E}_{max}$, $\|\tilde{F}_{n+1/2}\| \leq F_{max}$, where $\|\cdot\|$ is a given norm on V_h and*

$$\nu \leq x \cdot M(x + u_n). \quad (4.6)$$

Then there exists $\Delta t^ > 0$ depending on $\mathcal{E}_{max}$, F_{max} and ν such that, given $\Delta t \leq \Delta t^*$, τ_n , $\dot{\tau}_n$, θ_n , u_n and s_n , the external forces $f_{n+1/2}$ and $g_{n+1/2}$, there exists θ_{n+1} that satisfies (4.5) (with $u_{n+1/2}$ the corresponding solution of (4.4)).*

Moreover, there exists $\delta^+(\Delta t)$, $\delta^-(\Delta t)$ such that:

- $\lim_{\Delta t \rightarrow 0} \delta^+(\Delta t) = 2$,
- $\lim_{\Delta t \rightarrow 0} \delta^-(\Delta t) = -2$,
- $\theta_{n+1} \in [\theta_n + \delta^-(\Delta t), \theta_n + \delta^+(\Delta t)]$.

Proof. Given $\Delta t > 0$, $\eta \in]0, 1[$ and $\delta \in L := [-2 - \eta, 2 + \eta]$, we denote by $u(\delta, \Delta t) := u_{n+1/2}$ the solution of (4.4) corresponding to $\theta_{n+1} - \theta_n = \delta$. Since $\tilde{G}(\delta, 0)$ is invertible for $\delta \in L$, there exists Δt_0 (depending only on S), such that $\tilde{G}(\delta, \Delta t)$ is invertible on $L \times [0, \Delta t_0]$. Then, let us define $q(\delta, \Delta t)$ by:

$$q(\delta, \Delta t) := \Pi x \cdot \tilde{G}(\delta, \Delta t)^{-1} \Pi x.$$

The inversion of (4.4) provides:

$$u(\delta, \Delta t) = \tilde{G}(\delta, \Delta t)^{-1} \left(\tilde{c}_{n+1/2}(\delta, \Delta t) - \frac{1}{q(\delta, \Delta t)} \left((\Pi x) \cdot \tilde{G}(\delta, \Delta t)^{-1} \tilde{c}_{n+1/2}(\delta, \Delta t) \right) \Pi x \right).$$

By means of (4.6), we get, for $\delta \neq 0$:

$$(\Pi x) \cdot \tilde{G}(\delta, 0)^{-1} \tilde{c}_{n+1/2}(\delta, 0) = -\frac{2\delta}{(4 + \delta^2)^2} x \cdot M(x + u_n) \neq 0.$$

There exists $\Delta t'_0$ depending on $\mathcal{E}_{max}$, F_{max} and ν such that:

$$\forall(\delta, \Delta t) \in \{[-2 - \eta, -2 + \eta] \cup [2 - \eta, 2 + \eta]\} \times [0, \Delta t'_0], \\ (\Pi x) \cdot \tilde{G}(\delta, \Delta t)^{-1} \tilde{c}_{n+1/2}(\delta, \Delta t) \neq 0. \quad (4.7)$$

Let us focus now on the behavior of $q(\cdot, \cdot)$ on $\{[-2 - \eta, -2 + \eta] \cup [2 - \eta, 2 + \eta]\} \times [0, \Delta t'_0]$. One has:

$$q(\delta, 0) = \frac{4 - \delta^2}{(4 + \delta^2)^2} x \cdot Mx,$$

so that $q(-2, 0) = q(2, 0) = 0$ and $q(\delta, 0) \neq 0$ for $\delta \neq \pm 2$. Moreover, since:

$$\frac{\partial q}{\partial \delta}(\pm 2, 0) = \mp \frac{1}{16} x \cdot Mx \neq 0,$$

the implicit function theorem proves the existence of $\Delta t_0''$ (depending only on S) and two functions δ^+ and δ^- defined on $[0, \Delta t_0'']$ such that:

$$\begin{aligned} \forall \Delta t \in [0, \Delta t_0''], \quad q(\delta^+(\Delta t), \Delta t) &= 0, \quad q(\delta^-(\Delta t), \Delta t) = 0, \\ \lim_{\Delta t \rightarrow 0} \delta^-(\Delta t) &= -2, \quad \lim_{\Delta t \rightarrow 0} \delta^+(\Delta t) = 2. \end{aligned}$$

We have then proved the existence of two roots of $\delta \mapsto q(\delta, \Delta t)$ in L for all $\Delta t \leq \Delta t_0''$. By decreasing $\Delta t_0''$, these two roots can be guaranteed to be unique: indeed, suppose that there exists a sequence $(\Delta t_n)_{n \in \mathbb{N}}$ of $[0, \Delta t_0'']$ converging towards 0 and $(r_n)_{n \in \mathbb{N}}$ a sequence of roots of $h(\cdot, \Delta t_n)$ such that:

$$\forall n \in \mathbb{N}, \quad r_n \neq \delta^+(\Delta t_n), \quad r_n \neq \delta^-(\Delta t_n).$$

Since L is compact, we can assume that $(r_n)_{n \in \mathbb{N}}$ is convergent. By continuity of $q(\cdot, \cdot)$, the possible limits are -2 and 2 . Suppose for example that

$$\lim_{n \rightarrow +\infty} r_n = 2,$$

then

$$\lim_{n \rightarrow \infty} \frac{q(\delta^+(\Delta t_n), \Delta t_n) - q(r_n, \Delta t_n)}{\delta^+(\Delta t_n) - r_n} = 0 = \frac{\partial q}{\partial \delta}(2, 0) \neq 0,$$

which gives a contradiction. The case $\lim_{n \rightarrow +\infty} r_n = -2$ is similar.

Thanks to (4.7), we thus obtain that for $\Delta t \leq \Delta t^* := \min(\Delta t_0, \Delta t_0', \Delta t_0'')$, the function $\phi : \delta \mapsto u(\delta, \Delta t) \cdot Mu(\delta, \Delta t)$ satisfies:

- ϕ is continuous on $L - \{\delta^-(\Delta t), \delta^+(\Delta t)\}$,
- $\lim_{\delta \rightarrow \delta^-(\Delta t)} \phi(\delta) = \lim_{\delta \rightarrow \delta^+(\Delta t)} \phi(\delta) = +\infty$.

Since $h(\delta, \Delta t) = 4\delta\phi(\delta) + a_{n+1/2}(\delta) \cdot u(\delta, \Delta t) + b_{n+1/2}(\delta)$, where $a_{n+1/2}$ and $b_{n+1/2}$ are bounded on L , the existence of θ_{n+1} follows. $\square$

Remark: Note that the hypothesis (4.6) is the discretized version of the one of Theorem 2.1 and relies on the fact that the model is only valid for motions close to the rigid body motion, whereas the parameters F_{max} and $\mathcal{E}_{max}$ come from the discretization.

5. Extension to the 3D-case. This section is devoted to the extension of Algorithm II to the 3D-case. Here the rotation is parametrized by a vector. As a consequence, Algorithm I cannot be extended to 3D since it strongly relies on the scalar nature of the angular parameter, see, e.g., Equation (3.8).

The subset Ω is now a domain in $\mathbb{R}^3$. We denote by $\times$ the cross-product defined by:

$$\begin{pmatrix} a \\ b \\ c \end{pmatrix} \times \begin{pmatrix} a' \\ b' \\ c' \end{pmatrix} := \begin{pmatrix} bc' - b'c \\ a'c - ac' \\ ab' - a'b \end{pmatrix}.$$

5.1. Parametrization of 3D rotations. The major problem met when extending Algorithm II to 3D is to parametrize the rotation corresponding to the previous R_θ . We choose to describe it by using the Euler angles and refer to Appendix A of [18] for a review on other parametrizations. Given $\theta \in \mathbb{R}$, let us introduce R_θ^1 , R_θ^2 and R_θ^3 three rotation matrices defined by:

$$R_\theta^1 := \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \theta & -\sin \theta \\ 0 & \sin \theta & \cos \theta \end{pmatrix}, \quad R_\theta^2 := \begin{pmatrix} \cos \theta & 0 & -\sin \theta \\ 0 & 1 & 0 \\ \sin \theta & 0 & \cos \theta \end{pmatrix},$$

$$R_\theta^3 := \begin{pmatrix} \cos \theta & -\sin \theta & 0 \\ \sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

We also define for $i = 1, 2, 3$ the matrices $\Pi^i := \frac{1}{2}(R_{\frac{\pi}{2}}^i - R_{-\frac{\pi}{2}}^i)$.

Consider now $\theta = (\theta_1, \theta_2, \theta_3) \in \mathbb{R}^3$. We can now define the general 3D rotation matrix R_θ as follows:

$$R_\theta := R_{\theta_1}^1 R_{\theta_2}^2 R_{\theta_3}^3.$$

Suppose that θ depends on the time variable t , the derivative of R_θ reads:

$$\dot{R}_\theta = R_\theta \Theta^\theta(t),$$

where $\Theta^\theta(t)$ is the skew-symmetric matrix defined by:

$$\Theta^\theta(t) := \dot{\theta}_1(t)(R_{\theta_3(t)}^3)^\top (R_{\theta_2(t)}^2)^\top \Pi^1 R_{\theta_3(t)}^3 R_{\theta_2(t)}^2 + \dot{\theta}_2(t)(R_{\theta_3(t)}^3)^\top \Pi^2 R_{\theta_3(t)}^3 + \dot{\theta}_3(t) \Pi^3. \quad (5.1)$$

Note that $\Theta^\theta(t)$ depends both on $\theta(t)$ and $\dot{\theta}(t)$, hence our notation.

5.2. Model. Before considering the system of equations describing the dynamic, we introduce the space $\tilde{X} = \tilde{X}^{\text{trans}} \cap \tilde{X}^{\text{rot}}$ corresponding to X , defined by:

$$\tilde{X}^{\text{trans}} := \left\{ u \in \tilde{V}; \int_{\Omega} \rho u = 0 \right\}, \quad \tilde{X}^{\text{rot}} := \left\{ u \in \tilde{V}; \int_{\Omega} \rho u \times x = 0 \right\},$$

where $\tilde{V} := [H^1(\Omega)]^3$.

Let us now consider the time derivatives of the deformation φ . As for the 2D-case, we decompose it as:

$$\varphi(x, t) = \tau(t) + R_\theta(t)(x + u(x, t)),$$

where $\tau(t) \in \mathbb{R}^3$ and $u \in \tilde{X}$.

Introducing the relative velocity s defined by

$$s(x, t) := \dot{u}(x, t) + \Theta^\theta(t)(x + u(x, t)),$$

we obtain:

$$\dot{\varphi}(x, t) = \dot{\tau}(t) + R_{\theta(t)} s(x, t).$$

and

$$\ddot{\varphi}(x, t) = \ddot{\tau}(t) + R_{\theta(t)} \left(\dot{s}(x, t) + \Theta^\theta(t) s(x, t) \right).$$

The angular momentum is:

$$\mathcal{J} := R_\theta \int_{\Omega} \rho s \times (x + u).$$

Note that, in contrast to the 2D-case, we have to keep the rotation in this definition, since $\int_{\Omega} \rho s \times (x + u)$ cannot be colinear to the axis of the rotation. This fact motivates the introduction of the relative angular momentum defined by:

$$m := \int_{\Omega} \rho s \times (x + u).$$

In terms of m , the time derivative of $\mathcal{J}$ reads:

$$\dot{\mathcal{J}} = R_{\theta}(\dot{m} + \Theta^{\theta} m).$$

The dynamic of our system can be described by the following three equations:

$$\mathcal{M}\ddot{\tau} = \int_{\Omega} f + \int_{\Gamma} g,$$

$$\dot{m} + \Theta^{\theta} m = \int_{\Omega} R_{\theta}^{\top} f \times (x + u) + \int_{\Gamma} R_{\theta}^{\top} g \times (x + u)$$

and

$$\int_{\Omega} \rho(\dot{s} + \Theta^{\theta} s) \cdot v + \int_{\Omega} \sigma(u) : \varepsilon(v) = F_{\theta}(v), \quad \forall v \in \tilde{X},$$

where:

$$F_{\theta}(v) := \int_{\Omega} f \cdot R_{\theta} v + \int_{\Gamma} g \cdot R_{\theta} v.$$

5.3. 3D Algorithm. We are now in the position to extend Algorithm II to the 3D-case. We keep the notation corresponding to the mid-point time discretization, see (3.4).

Given $\tau_0, \dot{\tau}_0, \theta_0, u_0, s_0$, the external forces $(f_{n+1/2})_{n \in \mathbb{N}}$ and $(g_{n+1/2})_{n \in \mathbb{N}}$, and suppose that $\tau_n, \dot{\tau}_n, \theta_n, u_n \in \tilde{X}$ and s_n have already been computed. The derivation of $\tau_{n+1}, \dot{\tau}_{n+1}, \theta_{n+1}, u_{n+1} \in \tilde{X}$ and $s_{n+1} \in \tilde{V}$ is carried out by the resolution of:

$$\mathcal{M}\ddot{\tau}_{n+1/2} = \int_{\Omega} f_{n+1/2} + \int_{\Gamma} g_{n+1/2}, \quad (5.2)$$

$$\begin{aligned} K(\dot{m}_{n+1/2}, m_{n+1/2}, \dot{\theta}_{n+1/2}, \theta_{n+1/2}) &= \int_{\Omega} R_{\theta_{n+1/2}}^{\top} f_{n+1/2} \times (x + u_{n+1/2}) \\ &\quad + \int_{\Gamma} R_{\theta_{n+1/2}}^{\top} g_{n+1/2} \times (x + u_{n+1/2}), \end{aligned} \quad (5.3)$$

$$G(\dot{s}_{n+1/2}, s_{n+1/2}, \dot{\theta}_{n+1/2}, \theta_{n+1/2}, u_{n+1/2}; v) = F_{n+1/2}(v) \quad \forall v \in \tilde{X}, \quad (5.4)$$

with

$$\begin{aligned} K(\dot{m}, m, \dot{\theta}, \theta) &:= \dot{m} + \Theta^{\theta} m, \\ G(\dot{s}, s, \dot{\theta}, \theta, u; v) &:= \int_{\Omega} \rho(\dot{s} + \Theta^{\theta} s) \cdot v + \int_{\Omega} \sigma(u) : \varepsilon(v), \\ F_{n+1/2}(v) &:= \int_{\Omega} f_{n+1/2} \cdot R_{\theta_{n+1/2}} v + \int_{\Gamma} g_{n+1/2} \cdot R_{\theta_{n+1/2}} v, \end{aligned}$$

and

$$m_{n+1/2} := \int_{\Omega} \rho s_{n+1/2} \times (x + u_{n+1/2}), \quad s_{n+1/2} := \dot{u}_{n+1/2} + \Theta_{n+1/2}^{\theta} (x + u_{n+1/2}). \quad (5.5)$$

Here, $\Theta_{n+1/2}^{\theta}$ is the time discretization of $\Theta^{\theta}(t_{n+1/2})$ computed with $\theta_{n+1/2}$ and $\dot{\theta}_{n+1/2}$ by (5.1).

5.4. Angular momentum and energy conservation. As it was the case for Algorithm II, the 3D Algorithm preserves both the norm of the angular momentum and energy.

THEOREM 5.1. *The 3D Algorithm defined by (5.2)–(5.4) guarantees the energy conservation in the sense that:*

$$\mathcal{E}_{n+1} - \mathcal{E}_n = \Delta t \left(\int_{\Omega} f_{n+1/2} \cdot \dot{\varphi}_{n+1/2} + \int_{\Gamma} g_{n+1/2} \cdot \dot{\varphi}_{n+1/2} \right),$$

where s is defined by (5.5) and $\mathcal{E}$ is the total energy defined by (3.5). The time discretization of $\dot{\varphi}$ is done by:

$$\dot{\varphi}_{n+1/2} := \dot{\tau}_{n+1/2} + R_{\theta_{n+1/2}} s_{n+1/2}.$$

The proof of energy conservation can be obtained by following the one of Theorem 3.1.

Note that we do not have exact angular momentum conservation since $\dot{\mathcal{J}}$ cannot be written as an explicit variation of a time discretization of $\mathcal{J}$ between two timesteps. As for Algorithm I in 2D, it is however possible to specify the local order with respect to Δt . Defining the time-discretized angular momentum $\mathcal{J}$ by:

$$\mathcal{J}_n := R_{\theta_n} m_n,$$

where θ_n, u_n and s_n are computed by the 3D Algorithm, it can be shown that there exists $C_{n+1/2}$, depending only on $\theta_{n+1/2}$, such that:

$$\begin{aligned} \|\mathcal{J}_{n+1} - \mathcal{J}_n - \Delta t \left(\int_{\Omega} f_{n+1/2} \times R_{\theta_{n+1/2}}(x + u_{n+1/2}) + \int_{\Gamma} g_{n+1/2} \times R_{\theta_{n+1/2}}(x + u_{n+1/2}) \right)\| \\ \leq C_{n+1/2} \Delta t^2, \end{aligned}$$

where $\|\cdot\|$ is a norm in $\mathbb{R}^3$. Moreover, the norm of the angular momentum is preserved in the sense that:

$$\begin{aligned} \mathcal{J}_{n+1}^2 - \mathcal{J}_n^2 = 2\Delta t \left(\int_{\Omega} f_{n+1/2} \times R_{\theta_{n+1/2}}(x + u_{n+1/2}) \cdot R_{\theta_{n+1/2}} m_{n+1/2} \right. \\ \left. + \int_{\Gamma} g_{n+1/2} \times R_{\theta_{n+1/2}}(x + u_{n+1/2}) \cdot R_{\theta_{n+1/2}} m_{n+1/2} \right). \end{aligned}$$

6. Numerical examples. In this section, we present some numerical examples which show the flexibility and efficiency of our method. We start with several two dimensional examples which are numerically studied using the energy- and momentum conserving Algorithm II. At the end, we present a 3D example.

In our 2D examples, we compare the co-rotational formulation using linear and nonlinear Saint Venant–Kirchhoff material law with the results of the standard nonlinear Saint Venant–Kirchhoff setting. To do so, we compute from the solution of the standard nonlinear setting in a postprocess the translation τ_n and rotation angle θ_n such that the minimization condition (2.5) is fulfilled, i.e.,

$$\tau_n := \int_{\Omega} \rho \varphi_n, \quad \int_{\Omega} \rho R_{\theta_n}^{\top} (\varphi_n - \tau_n) \cdot \Pi x = 0.$$

We then set $\dot{\tau}_{n+1/2} = \frac{\tau_{n+1} - \tau_n}{\Delta t}$ and $\dot{\theta}_{n+1/2} = \frac{\theta_{n+1} - \theta_n}{\Delta t}$.

FIG. 6.1. *Example 1. Left: grid, middle: initial condition for co-rotational formulation, right: initial condition for nonlinear formulation (deformation with factor 200, effective stress)*

FIG. 6.2. *Example 1. Deformed mesh and effective stress at time $t = 0, 0.1, 0.2, 0.3, 0.4$.*

As initial deformations, we use either $u_0 = 0$, i.e., $\varphi_0 = x$ or $u_0 = u_{\text{rot}}(\dot{\theta}_0)$ and $\varphi_0 = \varphi_{\text{rot}}(\dot{\theta}_0)$, respectively, where u_{rot} , φ_{rot} are the displacements of a body rotating with a given constant angular speed $\dot{\theta}_0$.

Given the rotational speed $\dot{\theta}_0$, we obtain $u_{\text{rot}}(\dot{\theta}_0)$ by solving the system

$$-(\dot{\theta}_0)^2 M(x + u_{\text{rot}}) + S u_{\text{rot}} = 0. \quad (6.1)$$

We note that multiplying (6.1) with Πx gives $M u_{\text{rot}} \cdot \Pi x = 0$ and thus $u_{\text{rot}} \in X_h$.

For the nonlinear material law, $\varphi_{\text{rot}}(\dot{\theta}_0)$ is given by the solution of

$$-(\dot{\theta}_0)^2 M \varphi_{\text{rot}} + S(\varphi_{\text{rot}} - x) = 0. \quad (6.2)$$

Here, $S(\cdot)$ denotes the discretized nonlinear elasticity operator.

The nonlinear equation (4.5), $h(\theta_{n+1} - \theta_n) = 0$ is solved for our examples using a Newton scheme. We note that the derivative $\frac{d}{d\theta} u_{n+1/2}$ can be computed by solving the system (4.4) with a modified right hand side.

6.1. Example 1: Rotating beam. In this example, we consider a beam that is rotating with a constant speed. The domain Ω is given by $[-0.5, 0.5] \times [-0.05, 0.05]$, see Figure 6.1, and the material parameters by $E = 1.62 \cdot 10^5$, $\nu = 0.2$ and $\rho = 1.0$.

We assume no boundary and no volume forces, i.e., $g = 0$ and $f = 0$. As initial rotation speed, we use $\dot{\theta}_0 = 20$. For the co-rotational setting, we use the initial displacement $u_0 = u_{\text{rot}}(\dot{\theta}_0)$ for the linear material law and $u_0 = \varphi_{\text{rot}}(\dot{\theta}_0) - x$ for the nonlinear material law and set $s_0 = \dot{\theta}_0 \Pi(x + u_0)$, $\theta_0 = 0$. $\dot{\tau}_0 = (1, 1)^\top$, $\tau_0 = (0, 0)^\top$. With these initial conditions, it is easy to verify that the solution of (3.13)–(3.12) is given by $\theta_n = n \Delta t \dot{\theta}_0$, $\dot{\theta}_n = \dot{\theta}_0$, $\tau_n = n \Delta t \dot{\tau}_0$, $\dot{\tau}_n = \dot{\tau}_0$, $u_n = u_0$, $s_n = s_0$.

For the standard nonlinear setting, we set $\varphi_0 = \varphi_{\text{rot}}(\dot{\theta}_0)$ and $\dot{\varphi}_0 = \dot{\theta}_0 \Pi \varphi_0$. As timesteps we use $\Delta t = 0.05, 0.01, 0.001$. We note that in our co-rotational formulation

FIG. 6.3. Example 1. Computed angular speed and number of iterations, co-rotational formulation vs. nonlinear approach with different timesteps

FIG. 6.4. Example 2. Deformed mesh and effective stress (co-rotational linear) at time t_n , $n = 0, 5, 10, 15, 20$.

the solution is independent of the choice of Δt . Moreover, only one Newton iteration is needed if the iteration is started with θ_{n+1} such that $\dot{\theta}_{n+1/2} = \dot{\theta}_n$ which is the correct solution. For the nonlinear setting, we observe an increasing number of Newton steps with increasing Δt , see Figure 6.3. It turns out that for large Δt the nonlinear approach is not able to handle the rotation correctly resulting in a wrong rotational speed.

6.2. Example 2: Rotation of a soft disc with no initial deformation. In this example, we consider a soft rotating disc. The domain Ω is given by a circle with radius $r = 1.0$ and the material parameters by $E = 500$, $\nu = 0.2$ and $\rho = 1.0$. We assume no boundary and volume forces. As initial conditions for the co-rotational setting, we use $\dot{\theta}_0 = 20$ and assume no initial deformation $u_0 = 0$. The initial speed is given by $s_0 = \dot{\theta}_0 \Pi x$ and the initial rotation angle by $\theta_0 = 0$. For the standard nonlinear setting, we have $\varphi_0 = x$, $\dot{\varphi}_0 = \dot{\theta}_0 \Pi x$. We assume zero translation, i.e., $\tau = (0, 0)^\top$, $\dot{\tau} = (0, 0)^\top$. As timesteps we use $\Delta t = 0.001$.

In Figure 6.4, the solution of the co-rotational linear setting at various timesteps is shown. The calculated angular speed for the co-rotational and standard nonlinear approaches is depicted in Figure 6.5. We observe that the co-rotational linear approach

FIG. 6.5. *Example 2. Angular speed using nonlinear, co-rotational-nonlinear and co-rotational formulation.*

FIG. 6.6. *Example 2. Energies for nonlinear, co-rotational-nonlinear and co-rotational formulation.*

fails to resolve the frequency of the solution. This is due to the linear material law which gives a wrong approximation of the elastic term for large deformations. However, the co-rotational nonlinear setting perfectly reproduces the results obtained by the full nonlinear setting.

When comparing the energies and angular momentum for the three formulations (Figure 6.6), we see that all settings yield energy and angular-momentum conservation.

FIG. 6.7. Example 3. Number of Newton iterations comparing standard nonlinear with co-rotational linear setting

FIG. 6.8. Example 3. Angular speed for nonlinear and co-rotational settings with different Δt

6.3. Example 3: Rotation of a hard disc with no initial deformation. In this example, we consider a rotating hard disc. The domain Ω is given by a circle with radius $r = 1.0$ and the material parameters by $E = 1.62 \cdot 10^5$, $\nu = 0.2$ and $\rho = 1.0$. We use the same initial and boundary conditions as in the previous example and the timesteps $\Delta t = 0.001, 0.005, 0.01, 0.02$.

In Figure 6.7, the necessary Newton steps per timestep for the standard nonlinear and the co-rotational setting using linear material law are shown. One can see that for small timesteps the nonlinear and the co-rotational setting both perform quite well. For larger timesteps the number of iterations using the standard nonlinear approach increases while the co-rotational formulation stays at low iteration numbers.

The angular speed $\dot{\theta}$ comparing the co-rotational linear/nonlinear setting with the standard nonlinear setting are depicted in Figure 6.8. We see that for large timesteps the time integration scheme is no longer able to handle the oscillations correctly. Moreover, the standard nonlinear approach gives a wrong average rotation speed. This points out the fact that the standard time integration scheme with a large

FIG. 6.9. *Example 4. Left: rotation angle and rotation speed, right: energy and angular moment.*

FIG. 6.10. *Example 4. Effective stress and deformation u (factor 200) at time $t = 0, 0.2, 0.4, 0.5$.*

timestep is not able to handle the rotation correctly even when using geometrically nonlinear material laws. Here, the co-rotational approach yields a good approximation of the rotation speed using both linearized and nonlinear material laws.

6.4. Example 4: Rotation of a beam under surface traction. In this example, we consider a rotating beam under surface traction. For such rotational problems, boundary forces normal or perpendicular to the rotated configuration are quite common. This leads to a boundary force $g = R_\theta g_{\text{rel}}$, where g_{rel} is the boundary force relative to the rotated configuration and θ is the actual rotation angle that can be defined, for example, by (2.5). This setting causes extra difficulties when solving with standard time integration schemes as the right hand side depends on the actual solution. However, in the co-rotational framework, this type of boundary condition can be modeled in a natural way and moreover gives a right hand side that is independent of the actual rotation.

We use the same setting and initial conditions as in Example 1 and a timestep of $\Delta t = 0.01$. Here, the surface traction is given by $g_{\text{rel}} = (0, -20)^\top$ on the right boundary and $g_{\text{rel}} = (0, 20)^\top$ on the left boundary. On the top and bottom, we assume no surface traction. The rotation angle and angular speed using the co-rotational linear framework are depicted on the left of Figure 6.9, and the energy and angular momentum are shown on the right. In Figure 6.10, the deformation u is plotted at various timesteps. We note that for this example the number of necessary Newton iterations is two for all timesteps

6.5. Example 5: Rotation of a 3D cube. In our last example, we demonstrate the usage of our algorithm for 3D problems. We model a rotating cube with constant rotation axis $(1, 1, 1)^\top$. We note that for this kind of rotation, R can be represented in terms of just one rotation angle. Moreover, the angular momentum is exactly preserved in this example as Algorithm II preserves the norm of the angular momentum. The domain is given by $[0, 1] \times [0, 1] \times [0, 1]$ and the material parameters by $E = 1.62 \cdot 10^5$, $\nu = 0.2$ and $\rho = 1.0$. As in Example 3, we use $\Delta t = 0.01$, an initial angular speed of 20 and zero initial displacement. The results for the angular

FIG. 6.11. 3D Example. Deformed mesh at time $t = 0, 0.05, 0.1, 0.15, 0.2, 0.25, 0.3$.

speed, moment and energy are similar to those of Example 3. The deformed mesh at various timesteps is presented in Figure 6.11.

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