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HHT- α and TR-BDF2 schemes for dynamic contact problems

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Abstract

This work focuses on the numerical performance of HHT- α and TR-BDF2 schemes for dynamic frictionless unilateral contact problems between an elastic body and a rigid obstacle. Nitsche's method, the penalty method, and the augmented Lagrangian method are considered to handle unilateral contact conditions. Analysis of the convergence of an opposed value of the parameter $\tilde{\alpha}$ for the HHT- α method is achieved. The mass redistribution method has also been tested and compared with the standard mass matrix. Numerical results for 1D and 3D benchmarks show the functionality of the combinations of schemes and methods used.

Key words: contact problem, Nitsche's method, augmented Lagrangian method, finite elements, elastodynamics, time-marching schemes.

MSC Classification: 65N12, 65N30, 74M15

1 Introduction

One of the main tools for computational solid mechanics is the finite element method. In the industry, contact problems are omnipresent, and many traditional methods cannot provide acceptable solutions in the context of elastodynamics: they are too influenced by parasitic oscillations or do not conserve energy. A difficulty is that this type of problem has a nonlinear boundary condition on the displacement field. Contact problems can be formulated weakly within the framework of variational or quasi-variational inequalities (see, e.g., [31, 34, 35, 46, 54]). Those are the very basis of most existing Finite Element Methods (FEM), which are discretization methods commonly used in engineering to compute approximate solutions, see, e.g.,

[24, 37, 39, 41, 42, 54, 58, 75, 76]. The main existing methods for discretizing the Signorini contact conditions are the method of penalization, mixed/mortar methods, Nitsche's method, or the augmented Lagrangian method. Improvements in the accuracy and numerical robustness of these simulations are always expected by industry and researchers.

Usually, the time-space discretization involves the problems of choosing: (i) the finite element space; (ii) the enforcement of the contact condition, and (iii) the time-stepping scheme.

The idea concerned in this work for treating the nonlinear boundary condition is to transfer the constrained optimization problems to an unconstrained problem or a sequence of unconstrained problems. This approach for contact problems in the static case is largely discussed by Kikuchi and Oden [54, 62, 63]. In the dynamic case, several schemes, e.g., (modified) Crank-Nicolson, Newmark, HHT schemes [2, 30, 51, 57], Paoli-Schatzman schemes [65, 66], or more recently [29], to mention a few, have already been considered and problems of spurious oscillations and numerical instabilities caused by artificial energy creation have been reported [56].

Nitsche's method was originally introduced for the treatment of the Dirichlet boundary conditions as a consistent method without additional Lagrangian multipliers [60]. In recent years, it has been introduced for contact problems. Firstly proposed for frictionless unilateral contact in linear elasticity as the classical symmetric version in [17] and as variants (symmetric, skew-symmetric, and non-symmetric) versions in [23]. Then, the frictional case was considered for Tresca friction in [13, 14, 25] and for Coulomb friction in [6, 19, 72], with several analyses of a posteriori error estimates [16, 38]. An extension to large strain bilateral contact has also been performed in [77]. The works on dynamic contact with Nitsche's method begin from [21, 22]. This method yields a well-posed semi-discrete problem in space (discretization in space by finite element method and continuous in time with the conservation of modified energy for the symmetric variant). Different time-marching schemes can then be applied to discretize in time: the explicit Verlet scheme in [26], for the implicit schemes, the θ -scheme and Newmark scheme in [15, 19, 20], and some IMEX schemes in [7]. A new "hybrid" scheme has also been introduced in [21, 22].

The idea of the augmented Lagrangian method (ALM) originated from Hestenes [44] and Powell [67] independently [68] and was finally established by Fortin, Glowinski, and Le Tallec [36, 37] and it adds an additional variable that represents the contact pressure (normal boundary stress). Like Nitsche's method, ALM is also a consistent method. A first implementation of this method for contact problems with Coulomb's friction law was established by Alart and Curnier [1] and in recent years, convergence analysis for several reformulations have been realized by Burman et al. [10]. A review of the static case for both essential and inequality boundary conditions can be found in [11]. In Burman et al. [9, 10, 40], the link between Nitsche and ALM is also emphasized. In fact, the methods are very similar: Nitsche involves fewer unknowns but ALM allows more flexibility to discretize the contact pressure. Few references can be found for applications in the dynamic case via the ALM (and finite element method). We can refer for instance the work of [50]. Other approaches include mixed methods (see e.g. [41, 75]) or active set methods [48], that have been proposed to solve a differential inclusion as a system of inequalities. However, such strategies lead to ill-posed space semi-discretized problems, with multiple solutions after impact [52, Lem. 8].

For structural dynamic problems, methods of time integration for second-order differential equations are required and different time-marching schemes have been largely applied. The HHT- α scheme is a classical and representative method for elastodynamic problems proposed by Hilber, Hughes, and Taylor [45]. This scheme has been proved to be an A-stable method for linear elastodynamic cases and is widely used for solving, e.g., the dynamic of systems of mass points, rigid bodies, or combined with finite element method. In recent years, analysis of the HHT- α method for nonlinear problems was attracting more attention [32], and for contact problems, this method has been tested with other methods such as pure contact or penalty [30, 57]. It can be considered as a general case of the family of Newmark schemes [59], and there exists the generalized- α method as a possible extension [27].

Another main scheme concerned in this work is the TR-BDF2 scheme (also known as the Bathe scheme [4]), which is an implicit scheme with 2 sub-steps: the first sub-step uses the trapezoidal rule and the second sub-step uses a three-point backward difference approximation. This scheme was proposed targeted to the nonlinear dynamic problems where the Crank-Nicolson method and the Wilson- θ method [5] may fail to provide a stable solution. It can also be considered an implicit predictor-corrector scheme.

In this work, we focus on the evolution of the impact of a linear elastic body and a rigid obstacle. We want particularly to study how to combine time-marching schemes as HHT- α and TR-BDF2 schemes with contact via Nitsche's method, and possibly with the mass redistribution method. For instance, these two kinds of schemes have not been applied with Nitsche's method or ALM. We then present some simulation results with 1D and 3D benchmarks using these different methods. By testing their performances, we are particularly interested in the influence of the numerical parameters, the parasitic oscillation associated with the contact surface due to the discontinuity in time, and the conservation or not of the total energy for the time-marching schemes. The new combinations applied in this work can eventually improve upon existing methods by providing better accuracy and numerical robustness for nonlinear (and non-regular) dynamic problems.

This paper is organized as follows. We first introduce the mathematical models treating the Signorini boundary conditions and the semi-discretization of the elastodynamic problem in Sect. 2. In Sect. 3, we present the two time-marching schemes (HHT- α and TR-BDF2 method) as well as some analysis on convergence for an opposed parameter $\tilde{\alpha}$ for HHT- α method. In Sect. 4, we are going to show three benchmarks, including a new 1D benchmark with an analytic solution, with their numerical simulations. Moreover, the mass redistribution method [28] has been applied and compared for the two 1D benchmarks, and the hybrid Nitsche scheme [22] has been tested with the 3D benchmark.

2 Contact problem and choosing of the enforcement of contact condition

We consider an elastic body $\Omega \subset \mathbb{R}^d$, $d \in \{1, 2, 3\}$, see Fig. 1. On the boundary $\partial \Omega := \Gamma_D \cup \Gamma_N \cup \Gamma_C$ of Ω , Dirichlet, Neumann, and Signorini boundary conditions are applied respectively on the

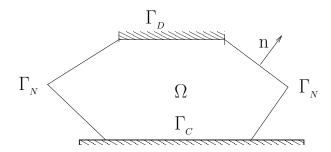


Figure 1: Elastic body occupying the domain Ω , with the boundary $\partial\Omega$.

disjoint subsets Γ_D , Γ_N , and Γ_C .

We seek the displacement field $\mathbf{u}: \Omega \times (0,T) \to \mathbb{R}^d$, where T > 0 is the final time, verifying the equations (1):

$$\rho \ddot{\mathbf{u}} - \operatorname{div}(\sigma(\mathbf{u})) = \mathbf{f}(t), \text{ in } \Omega \times (0, T), \qquad (i)$$

$$\sigma(\mathbf{u}) = \lambda \operatorname{tr}(\epsilon(\mathbf{u}))\mathbf{I} + 2\mu\epsilon(\mathbf{u}), \text{ in } \Omega \times (0, T), \qquad (ii)$$

$$\mathbf{u} = \mathbf{0}, \text{ on } \Gamma_D \times (0, T), \qquad (iii)$$

$$\sigma(\mathbf{u}) \cdot \mathbf{n} = \mathbf{f}_N(t), \text{ on } \Gamma_N \times (0, T), \qquad (iv)$$

$$u_n \leq 0, \quad \sigma_n(\mathbf{u}) \leq 0, \quad u_n \sigma_n(\mathbf{u}) = 0, \text{ on } \Gamma_C \times (0, T), \qquad (v)$$

$$\sigma(\mathbf{u}) \cdot \mathbf{n} - \sigma_n(\mathbf{u}) \cdot \mathbf{n} = \mathbf{0}, \text{ on } \Gamma_C \times (0, T), \qquad (vi)$$

$$\mathbf{u}(\cdot, 0) = \mathbf{u}_0, \quad \dot{\mathbf{u}}(\cdot, 0) = \dot{\mathbf{u}}_0, \text{ in } \Omega. \qquad (vii)$$

The equations (i) - (iv) describe the problem of elastodynamics in small deformation, where ρ is the mass density, $\mathbf{f}(t)$ is the volumetric source term, $\mathbf{f}_N(t)$ is the surface charge, λ and μ are Lamé coefficients, $\operatorname{tr}(\cdot)$ denotes the trace of a matrix, $\epsilon(\cdot) := \frac{1}{2} \left(\nabla(\cdot) + \nabla^T(\cdot) \right)$ is the deformation tensor and \mathbf{I} is the identity matrix of dimension d. The equations (v) and (vi) denote Signorini's condition for frictionless contact, where $u_n = \mathbf{u} \cdot \mathbf{n}$, $\sigma_n(\mathbf{u}) = (\sigma(\mathbf{u}) \cdot \mathbf{n}) \cdot \mathbf{n}$ are respectively the normal displacement and the contact pressure at boundary Γ_C . The initial conditions at the time t = 0 on the initial displacement and velocity fields are given in equation (vii). We also introduce the bilinear and linear forms

$$a(\mathbf{u}, \mathbf{v}) := (\sigma(\mathbf{u}), \epsilon(\mathbf{v}))_{\Omega}, l(t)(\mathbf{v}) := (\mathbf{f}(t), \mathbf{v})_{\Omega} + (\mathbf{f}_{N}(t), \mathbf{v})_{\Gamma_{N}},$$
(2)

where the notation $(\mathbf{u}, \mathbf{v})_{\Omega} := \int_{\Omega} \mathbf{u} \cdot \mathbf{v} \, d\Omega$ and $(\mathbf{u}, \mathbf{v})_{\Gamma_F} := \int_{\Gamma_F} \mathbf{u} \cdot \mathbf{v} \, d\Gamma$ are the L^2 -products defined on Ω and Γ_F respectively, with $\Gamma_F \in \{\partial\Omega, \Gamma_D, \Gamma_N, \Gamma_C\}$. The associated norms are denoted by $||\cdot||_{\Omega} := (\cdot, \cdot)_{\Omega}^{\frac{1}{2}}$ and $||\cdot||_{\Gamma_F} := (\cdot, \cdot)_{\Gamma_F}^{\frac{1}{2}}$.

Let V^h be the Lagrange finite element space to discretize the displacement, of degree one or two (k = 1 or 2), and based on a mesh \mathcal{T}^h of the domain Ω :

$$\mathbf{V}^{h} := \left\{ \mathbf{v}^{h} \in \left(C^{0}(\overline{\Omega}) \right)^{d} : \mathbf{v}_{|\Gamma_{D}}^{h} = \mathbf{0}; \ \mathbf{v}_{|T}^{h} = \mathbb{P}_{k}(T), \ \forall T \in \mathcal{T}^{h} \right\}.$$
 (3)

We also introduce the space W^h defined as the piecewise linear space on Γ_C for the continuous Lagrange multiplier used for the case k=2:

$$W^{h} := \left\{ \mu^{h} \in C^{0}(\overline{\Gamma_{C}}) : \mu^{h}_{|T \cap \Gamma_{C}} \in \mathbb{P}_{1}(T), \ \forall T \in \mathcal{T}^{h} \right\}. \tag{4}$$

The total mechanical energy associated with the solution \mathbf{u} of dynamic Signorini problem (1) is:

$$E(t) = \frac{1}{2} \left(\rho \dot{\mathbf{u}}, \dot{\mathbf{u}} \right)_{\Omega} + \frac{1}{2} a(\mathbf{u}, \mathbf{u}), \ \forall t \in [0, T].$$
 (5)

Moreover, with the persistency condition [2, 43, 57] $(\sigma(\mathbf{u}) \cdot \mathbf{n}) \cdot \dot{\mathbf{u}} = 0$ on Γ_C , and when l(t) vanishes, the evolution of energy

$$\frac{\mathrm{d}}{\mathrm{d}t}E(t) = 0$$

and the total mechanical energy is constant on time.

The enforcement of contact conditions is then introduced at the discrete level, with Nitsche's, penalty and ALM formulations.

2.1 Nitsche's method

Initially introduced by Nitsche [60] (see also [73]), the method has been extended by [17, 23] for the unilateral contact problem, then in elastodynamics [20, 21, 22]. We are going to define the space-discrete weak formulation of the Nitsche-FEM method: first, we introduce the linear discrete operator

$$P_N: \begin{array}{ccc} \mathbf{V}^h & \to & L^2(\Gamma_C) \\ \mathbf{v}^h & \mapsto & \sigma_n(\mathbf{v}^h) - \gamma_N v_n^h \end{array}, \tag{6}$$

where γ_N is a positive function independent of \mathbf{v} , such that

$$\gamma_{N|T\cap\Gamma_C} = \frac{\gamma_0}{h_T},\tag{7}$$

so for each triangle T intersected with Γ_C , where h_T is the diameter of the triangle T and γ_0 is a positive constant (the Nitsche parameter). The primal discrete problem is as follows:

$$\begin{cases}
\operatorname{Seek} \mathbf{u}^{h} : [0, T] \to \mathbf{V}^{h}, \text{ s.t.} \\
\left(\rho \ddot{\mathbf{u}}^{h}(t), \mathbf{v}^{h}\right)_{\Omega} + a_{\gamma_{N}}(\mathbf{u}^{h}(t), \mathbf{v}^{h}) + \left(\frac{1}{\gamma_{N}} \left[P_{N}(\mathbf{u}^{h}(t))\right]_{\mathbb{R}^{-}}, P_{N}(\mathbf{v}^{h})\right)_{\Gamma_{C}} = l(t)(\mathbf{v}), \ \forall \mathbf{v}^{h} \in \mathbf{V}^{h},
\end{cases} \tag{8}$$

where $a_{\gamma_N}(\mathbf{u}^h, \mathbf{v}^h) := a(\mathbf{u}^h, \mathbf{v}^h) - \left(\frac{1}{\gamma_N}\sigma_n(u^h), \sigma_n(v^h)\right)_{\Gamma_C}$. The notation $[\cdot]_{\mathbb{R}^-} := \min(0, \cdot)$ denotes the projection on the half-line formed by negative real numbers. The method is symmetric (non-symmetric and skew-symmetric versions also exist but are not considered here). Also, in static (or when $\rho = 0$), it is convergent and well-posed for γ_0 large enough. Subsequently, by using

Riesz's representation theorem, the mass operator $\mathbf{M}: \mathbf{V}^h \to \mathbf{V}^h$ and the nonlinear operator $\mathbf{B}_N: \mathbf{V}^h \to \mathbf{V}^h$ are defined such that

$$\left(\mathbf{M}(\mathbf{v}^{h}), \mathbf{w}^{h}\right)_{\Omega} = \left(\rho \mathbf{v}^{h}, \mathbf{w}^{h}\right)_{\Omega}, \ \forall \mathbf{w}^{h} \in \mathbf{V}^{h},
\left(\mathbf{B}_{N}(\mathbf{v}^{h}), \mathbf{w}^{h}\right) = a_{\gamma_{N}}(\mathbf{v}^{h}, \mathbf{w}^{h}) + \left(\frac{1}{\gamma_{N}} \left[P_{N}(\mathbf{v}^{h})\right]_{\mathbb{R}^{-}}, P_{N}(\mathbf{w}^{h})\right)_{\Gamma_{C}}, \ \forall \mathbf{w}^{h} \in \mathbf{V}^{h}.$$
(9)

The vector $\mathbf{L}(t) \in \mathbf{V}^h$ is then defined such that

$$\left(\mathbf{L}(t), \mathbf{w}^h\right)_{\Omega} = l(t)(\mathbf{w}^h), \ \forall \mathbf{w}^h \in \mathbf{V}^h.$$
 (10)

Then, the compact form of (8) is

$$\begin{cases} \operatorname{Seek} \mathbf{u}^{h} : [0, T] \to \mathbf{V}^{h}, \text{ s.t.} \\ \mathbf{M}\ddot{\mathbf{u}}^{h}(t) + \mathbf{B}_{N}(\mathbf{u}^{h}(t)) = \mathbf{L}(t), \\ \mathbf{u}^{h}(0) = \mathbf{u}_{0}^{h}, \quad \dot{\mathbf{u}}^{h}(0) = \dot{\mathbf{u}}_{0}^{h}, \end{cases}$$
(11)

which is a system of lipschitzien differential equations and its well-posedness has been proven in [21]. Let us define the discrete energy as follows:

$$E^{h}(t) := \frac{1}{2} \left(\rho \dot{\mathbf{u}}^{h}(t), \dot{\mathbf{u}}^{h}(t) \right)_{\Omega} + \frac{1}{2} a(\mathbf{u}^{h}(t), \mathbf{u}^{h}(t)), \tag{12}$$

which is associated to the solution $\mathbf{u}^h(t)$ to Problem (8). Note that this is the direct transposition of the mechanical energy E(t) for the continuous system. Set also

$$E_N^h(t) := E^h(t) - \frac{1}{2} \left\| \gamma_N^{-\frac{1}{2}} \sigma_n(\mathbf{u}^h(t)) \right\|_{\Gamma_C}^2 + \frac{1}{2} \left\| \gamma_N^{-\frac{1}{2}} \left[P_N(\mathbf{u}^h(t)) \right]_{\mathbb{R}^-} \right\|_{\Gamma_C}^2$$

$$:= E^h(t) - R_N^h(t),$$
(13)

which corresponds to a modified energy in which a consistent term is added. This term denoted $R_N^h(t)$ represents, roughly speaking, the nonfulfillment of the contact condition (1)(v) by $\mathbf{u}^h(t)$ [15, 21]. This modified energy E_N^h is conserved if (1) is conservative.

Note that, though the standard convergence analysis in the static case requires, for technical reasons, extra regularity assumptions [23], there is in fact no extra regularity required to write a Nitsche method (and the assumptions in [23] can be weakened in fact, see [33, 38]).

2.2 Penalty method

The discrete reformulation of the standard penalty method for the unilateral Signorini problem writes as follows:

$$\begin{cases}
\operatorname{Seek} \mathbf{u}_{\epsilon}^{h} : [0, T] \to \mathbf{V}^{h}, \text{ s.t.} \\
\left(\rho \ddot{\mathbf{u}}_{\epsilon}^{h}(t), \mathbf{v}^{h}\right)_{\Omega} + a(\mathbf{u}_{\epsilon}^{h}(t), \mathbf{v}^{h}) + \frac{1}{\epsilon} \left(\left[u_{\epsilon, n}^{h}(t)\right]_{\mathbb{R}^{+}}, v_{n}^{h}\right)_{\Gamma_{C}} = l(t)(\mathbf{v}^{h}), \forall \mathbf{v} \in \mathbf{V}^{h},
\end{cases}$$
(14)

where $[\cdot]_{\mathbb{R}+} = \max(0,\cdot)$ denotes the projection on $\mathbb{R}+$, and $\epsilon_{|T\cap\Gamma_C} = \epsilon_0 h_T$ for each T intersected with Γ_C , with ϵ_0 a positive constant. This problem (14) is well-posed [8, 18] but is non-consistent, in contrast to Nitsche's method. There also exists a generalized class of penalty models applied to the Signorini problem, the so-called normal compliance model, corresponding to a power-law regularization of the penalty methods [12, 55, 64].

We can also define a compact form as for Nitsche's method:

$$\begin{cases}
\operatorname{Seek} \mathbf{u}_{\epsilon}^{h} : [0, T] \to \mathbf{V}^{h} \text{ s.t.} \\
\mathbf{M}\ddot{\mathbf{u}}_{\epsilon}^{h}(t) + \mathbf{B}_{P}(\mathbf{u}_{\epsilon}^{h}(t)) = \mathbf{L}(t), \\
\mathbf{u}_{\epsilon}^{h}(0) = \mathbf{u}_{0}^{h}, \quad \dot{\mathbf{u}}_{\epsilon}^{h}(0) = \dot{\mathbf{u}}_{0}^{h},
\end{cases} \tag{15}$$

with the nonlinear operator $\mathbf{B}_P: \mathbf{V}^h \to \mathbf{V}^h$ defined using Riesz's theorem:

$$\left(\mathbf{B}_{P}(\mathbf{v}^{h}), \mathbf{w}^{h}\right) = a(\mathbf{v}^{h}, \mathbf{w}^{h}) + \left(\frac{1}{\epsilon} \left[v_{n}^{h}\right]_{\mathbb{R}^{+}}, w_{n}^{h}\right)_{\Gamma_{C}}, \ \forall \mathbf{w} \in \mathbf{V}^{h}.$$
 (16)

The modified energy associated with the penalty method is the following one [26, 43]:

$$E_P^h(t) := E^h(t) + \frac{1}{2} \left\| e^{-\frac{1}{2}} \left[u_n^h(t) \right]_{\mathbb{R}^+} \right\|_{\Gamma_C}^2. \tag{17}$$

2.3 Augmented Lagrangian

The augmented Lagrangian method has been proposed as a penalty-duality formulation [1]. We first introduce the bi-linear form $P_A(\mathbf{u}, \lambda) = \lambda - \gamma_A u_n$, and the contact pressure can be reformulated as $\lambda = [P_A(\mathbf{u}, \lambda)]_{\mathbb{R}^-}$ [73], where γ_A is a positive parameter. In this work, γ_A is taken similarly to γ_N as $\gamma_{A|T\cap\Gamma_C} = \frac{\gamma_a}{h_T}$ for each T intersected with Γ_C and with γ_a a positive constant. Different formulations for contact problems in the static case have been introduced [10]. In this work, we focus on the following augmented Lagrangian reformulation:

$$\begin{cases}
\operatorname{Seek} \left(\mathbf{u}^{h}, \lambda^{h}\right) : [0, T] \to \mathbf{V}^{h} \times W^{h}, \text{ s.t.} \\
\left(\rho \ddot{\mathbf{u}}^{h}(t), \mathbf{v}^{h}\right)_{\Omega} + a(\mathbf{u}^{h}(t), \mathbf{v}^{h}) - \left(\left[P_{A}(\mathbf{u}^{h}(t), \lambda^{h}(t))\right]_{\mathbb{R}^{-}}, v_{n}^{h}\right)_{\Gamma_{C}} = l(t)(\mathbf{v}^{h}), \quad \forall \mathbf{v}^{h} \in \mathbf{V}^{h}, \\
\left(\frac{1}{\gamma_{A}} \left(\left[P_{A}(\mathbf{u}^{h}(t), \lambda^{h}(t))\right]_{\mathbb{R}^{-}} - \lambda^{h}(t)\right), \mu^{h}\right)_{\Gamma_{C}} = 0, \quad \forall \mu^{h} \in W^{h}.
\end{cases}$$
(18)

The stability of (18) with conditions in the static case (or when $\rho = 0$) for a scalar field has been proven by [10, Sect. 4]. This reformulation is also known as the proximal ALM, and the relation with Nitsche's method (8) can be obtained by interpreting λ^h as $\sigma_n(\mathbf{u}^h)$.

Similar to Nitsche's method and the penalty method, we can write a compact form:

$$\begin{cases}
\operatorname{Seek} (\mathbf{u}^h, \lambda^h) : [0, T] \to \mathbf{V}^h \times W^h \text{ s.t.} \\
\mathbf{M}\ddot{\mathbf{u}}^h(t) + \mathbf{B}_A(\mathbf{u}^h(t), \lambda^h(t)) = \mathbf{L}(t), \\
\mathbf{u}^h(0) = \mathbf{u}_0^h, \quad \dot{\mathbf{u}}^h(0) = \dot{\mathbf{u}}_0^h,
\end{cases} (19)$$

with nonlinear operator $\mathbf{B}_A: \mathbf{V}^h \times W^h \to \mathbf{V}^h \times W^h$ defined using Riesz's theorem:

$$\left(\mathbf{B}_{A}(\mathbf{v}^{h}, \mu^{h}), (\mathbf{w}^{h}, \xi^{h})\right) = a(\mathbf{v}^{h}, \mathbf{w}^{h}) + \left(\frac{1}{\gamma_{A}} \left[P_{A}(\mathbf{v}^{h}, \mu^{h})\right]_{\mathbb{R}^{-}}, P_{A}(\mathbf{w}^{h}, \xi^{h})\right)_{\Gamma_{C}} - \left(\frac{1}{\gamma_{A}} \mu^{h}, \xi^{h}\right)_{\Gamma_{C}}, \ \forall \ (\mathbf{w}^{h}, \xi^{h}) \in \mathbf{V}^{h} \times W^{h}.$$
(20)

The modified energy $E_L^h(t)$ can be set as:

$$E_L^h(t) := E^h(t) - \frac{1}{2} \left\| \gamma_A^{-\frac{1}{2}} \lambda^h(t) \right\|_{\Gamma_C}^2 + \frac{1}{2} \left\| \gamma_A^{-\frac{1}{2}} \left[P_A(\mathbf{u}^h(t), \lambda^h(t)) \right]_{\mathbb{R}^-} \right\|_{\Gamma_C}^2$$

$$:= E^h(t) - R_L^h(t).$$
(21)

2.4 Elastodynamic and mass redistribution method

For penalty or Nitsche's method, we have the semi-discrete problem defined in the form

$$\begin{cases}
\operatorname{Seek} \mathbf{u}^{h} : [0, T] \to \mathbf{V}^{h} \text{ s.t.} \\
\mathbf{M}\ddot{\mathbf{u}}^{h}(t) + \mathbf{B}(\mathbf{u}^{h}(t)) = \mathbf{L}(t), \\
\mathbf{u}^{h}(0) = \mathbf{u}_{0}^{h}, \quad \dot{\mathbf{u}}^{h}(0) = \dot{\mathbf{u}}_{0}^{h},
\end{cases} (22)$$

where **B** is equal to \mathbf{B}_P , or \mathbf{B}_N , for penalty, or Nitsche's method, respectively. And, for ALM:

$$\begin{cases}
\operatorname{Seek} (\mathbf{u}^h, \lambda^h) : [0, T] \to \mathbf{V}^h \times W^h \text{ s.t.} \\
\mathbf{M}\ddot{\mathbf{u}}^h(t) + \mathbf{B}_A(\mathbf{u}^h(t), \lambda^h(t)) = \mathbf{L}(t), \\
\mathbf{u}^h(0) = \mathbf{u}_0^h, \quad \dot{\mathbf{u}}^h(0) = \dot{\mathbf{u}}_0^h
\end{cases} \tag{23}$$

A large part of the numerical instabilities for simulations of dynamic contact problems come from the strong discontinuity of acceleration at the contact boundary. A novel idea is the mass redistribution method which conserves the total mass, the center of gravity, and the inertia momenta, but is built so that there is no inertia for the contact nodes [28, 53]. Moreover, the redistributed mass matrix \mathbf{M}^r shares an identical sparse structure with \mathbf{M} , (only with more zeros for contact nodes). An example of a comparison of different mass matrices on a 1D bar occupying $\Omega = (0,1)$ meshed uniformly with 20 linear elements is illustrated in Fig. 2, with contact boundary at x = 0 and Dirichlet boundary at x = 1. Each cross represents a node with its mass valued on the y-axis: the mass is uniformly distributed (except the two nodes on the two sides which possess only half as in the middle); while for the redistributed mass matrix, the node at x = 0 has a zero-mass and its initial mass has been redistributed to other nodes.

3 Discretization in time

In this work, we are especially interested in two families of time-marching schemes: the HHT- α scheme and the TR-BDF2 scheme.

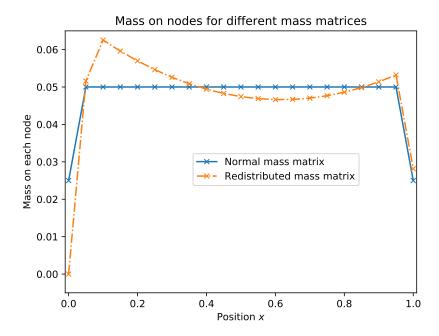


Figure 2: Comparison of different mass matrices on linear 1D elements.

3.1 Hilber-Hughes-Taylor- α (HHT- α) scheme

The HHT- α scheme [45] is a classical scheme for elastodynamic problems. Let $\Delta t > 0$ be the time-step and consider a uniform discretization of the time interval $[0,T]:(t^0,\cdots,t^N)$, with $t^n = n\Delta t, n = 0,\cdots,N$. This scheme consists of solving a nonlinear problem for each time instant t^{n+1} using the displacement $\mathbf{u}^{h,n}$, velocity $\dot{\mathbf{u}}^{h,n}$, and acceleration $\ddot{\mathbf{u}}^{h,n}$ of instant t^n as known variables:

$$\begin{cases}
\operatorname{Seek} \mathbf{u}^{h,n+1}, \dot{\mathbf{u}}^{h,n+1}, \ddot{\mathbf{u}}^{h,n+1} \in \mathbf{V}^{h} \text{ s.t.} \\
\mathbf{u}^{h,n+1} = \mathbf{u}^{h,n} + \Delta t \dot{\mathbf{u}}^{h,n} + \frac{\Delta t^{2}}{2} ((1 - 2\tilde{\beta}) \ddot{\mathbf{u}}^{h,n} + 2\tilde{\beta} \ddot{\mathbf{u}}^{h,n+1}), & \text{(i)} \\
\dot{\mathbf{u}}^{h,n+1} = \dot{\mathbf{u}}^{h,n} + \Delta t ((1 - \tilde{\gamma}) \ddot{\mathbf{u}}^{h,n} + \tilde{\gamma} \ddot{\mathbf{u}}^{h,n+1}), & \text{(ii)} \\
\mathbf{M} \ddot{\mathbf{u}}^{h,n+1} + (1 - \tilde{\alpha}) \mathbf{B} (\mathbf{u}^{h,n+1}) + \tilde{\alpha} \mathbf{B} (\mathbf{u}^{h,n}) = (1 - \tilde{\alpha}) \mathbf{L}^{n+1} + \tilde{\alpha} \mathbf{L}^{n}, & \text{(iii)}
\end{cases}$$

where $\mathbf{u}^{h,n+1}$, $\dot{\mathbf{u}}^{h,n+1}$, and $\ddot{\mathbf{u}}^{h,n+1}$ are the displacement, velocity, and acceleration to be solved. The parameter $\tilde{\alpha}$ allows a dissipation for high frequencies. The scheme parameters $(\tilde{\alpha}, \tilde{\beta}, \tilde{\gamma})$ are often related in practice. A classical combination of the parameters is $\tilde{\alpha} \in \left[0, \frac{1}{3}\right]$, $\tilde{\beta} = \frac{1}{4}(1+\tilde{\alpha})^2$, $\tilde{\gamma} = \frac{1}{2} + \tilde{\alpha}$. Such a choice of parameters yields unconditional stability for linear elasticity and the scheme is implicit. Notably, for $\tilde{\alpha} = 0$, the scheme is also known as the Crank-Nicolson scheme or a scheme of the Newmark family with $\tilde{\beta} = \frac{1}{4}$ and $\tilde{\gamma} = \frac{1}{2}$ (or the implicit

trapezoidal method). In this case, the scheme conserves the energy in the linear elastic domain without contact and has a second-order accuracy. But with the presence of contact, it can be more complicated and can introduce additional oscillations and numerical energy [22].

Larger values of $\tilde{\alpha}$ help filter more oscillation on high frequencies, however, it dissipates also more energy so we might lose the reliability at an industrial point. We would like to provide a possible value of the parameter that allows an acceptable compromise between parasitic oscillation and the loss of energy.

3.2 Possibility of opposed parameter

A positive value for the parameter $\tilde{\alpha}$ (with $\tilde{\beta} = \frac{1}{4}(1+|\tilde{\alpha}|)^2$ and $\tilde{\gamma} = \frac{1}{2}+|\tilde{\alpha}|$ in order to keep the values of $\tilde{\beta}$ and $\tilde{\gamma}$ remaining in the unconditionally stable region), representing an interpolation of the external and internal force can provide dissipation of energy of high frequencies. Moreover, we found that an extrapolation realized with a negative value can also provide a similar effect. We detail this point below with a stability and consistency analysis. Consider a single-degree-of-freedom (SDOF) oscillator

$$\begin{cases}
m\ddot{u} + ku = 0, t \in (0, T), \\
u(0) = u^{0}, \dot{u}(0) = \dot{u}^{0}.
\end{cases}$$
(25)

Let u = u(t) be the exact solution and $u^n, \dot{u}^n, \ddot{u}^n$ the approximate values at time $t^n = n\Delta t, n \in \mathbb{N}$. For a one-step method, we can define a corresponding continuous operator $\Phi_{\Delta t} : [0, T] \times \mathbb{R}^3 \to \mathbb{R}$ depending on the time-step Δt , [74] so that u^{n+1} can be calculated by:

$$u^{n+1} = u^n + \Delta t \Phi_{\Delta t}(t^n, u^n, \dot{u}^n, \ddot{u}^n), \tag{26}$$

and the associated local truncation error [49, 71, 74] is:

$$T_n := \frac{u(t^{n+1}) - u(t^n)}{\Delta t} - \Phi_{\Delta t}(t^n, u(t^n), \dot{u}(t^n), \ddot{u}(t^n)). \tag{27}$$

Applying to the SDOF system (25), the error is then bounded (see Sect. A.1 for details):

$$|T_n| \leq \tilde{\beta} \left| \omega^2 u(t^n) + \ddot{u}(t^n) \right| \Delta t + \tilde{\beta} \left(1 - \tilde{\alpha} \right) \omega^2 \left| \dot{u}(t^n) \right| \Delta t^2 + O(\Delta t^2)$$

$$= \tilde{\beta} \left(1 - \tilde{\alpha} \right) \omega^2 \left| \dot{u}(t^n) \right| \Delta t^2 + O(\Delta t^2), \tag{28}$$

with $\omega^2 = \frac{k}{m}$. And a second-order convergence is achieved.

3.2.1 Analysis of spectral radius

Let us rewrite the discrete problem of system (25) in matrix form (see Sect. A.2 for the expression of matrix \mathbf{A}):

$$\mathbf{Y}^{n+1} = \mathbf{A}\mathbf{Y}^n,\tag{29}$$

where $\mathbf{Y}^n = [u^n, \Delta t \dot{u}^n, \Delta t^2 \ddot{u}^n]^T$ and \mathbf{A} is the amplification matrix. The spectral radius of \mathbf{A} is defined by:

$$\rho(\mathbf{A}) = \max_{1 \le i \le 3} |\lambda_i|,\tag{30}$$

where $\lambda_i, i \in \{1, 2, 3\}$, are the eigenvalues of **A**. The condition $\rho(\mathbf{A}) \leq 1$ is equivalent to the unconditional stability of the scheme irrespectively to the time-step, for linear boundary conditions.

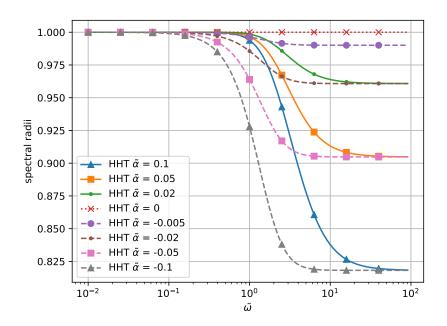


Figure 3: Spectral radii for HHT- α scheme vs frequencies for different $\tilde{\alpha}$.

We illustrate the spectral radii for the HHT- α scheme with different values of parameter $\tilde{\alpha}$ in Fig.3. The spectral radii show a dissipation for high frequencies and a negative $\tilde{\alpha}$ dissipates more at lower frequencies than its positive counterpart. Moreover, it can be observed that the spectral radii tend to have the same value when $\tilde{\omega} := \omega^2 \Delta t^2 \to \infty$ for opposite $\tilde{\alpha}$ but with the same absolute value. In fact, when $\tilde{\omega} \to \infty$,

$$\lim_{\tilde{\omega} \to \infty} \mathbf{A} = \begin{bmatrix} \frac{-\tilde{\alpha}}{1-\tilde{\alpha}} & 0 & 0\\ \frac{\tilde{\gamma}}{\tilde{\beta}} \begin{pmatrix} -\tilde{\alpha}\\ 1-\tilde{\alpha} \end{pmatrix} & 1 - \frac{\tilde{\gamma}}{\tilde{\beta}} & 1 - \frac{\tilde{\gamma}}{2\tilde{\beta}}\\ \frac{1}{\tilde{\beta}} \begin{pmatrix} -\tilde{\alpha}\\ 1-\tilde{\alpha} \end{pmatrix} & -\frac{1}{\tilde{\beta}} & \frac{2\tilde{\beta}-1}{2\tilde{\beta}} \end{bmatrix}, \tag{31}$$

which has the following eigenvalues:

$$\begin{cases}
\lambda_{1} = \frac{-\tilde{\alpha}}{1 - \tilde{\alpha}}, \\
\lambda_{2} = \frac{4\tilde{\beta} - 2\tilde{\gamma} - 1}{4\tilde{\beta}} - \sqrt{\frac{-16\tilde{\beta} + 4\tilde{\gamma}^{2} + 4\tilde{\gamma} + 1}{4\tilde{\beta}}}, \\
\lambda_{3} = \frac{4\tilde{\beta} - 2\tilde{\gamma} - 1}{4\tilde{\beta}} + \sqrt{\frac{-16\tilde{\beta} + 4\tilde{\gamma}^{2} + 4\tilde{\gamma} + 1}{4\tilde{\beta}}}.
\end{cases} (32)$$

With respect to the relation between $\tilde{\alpha}$, $\tilde{\beta}$ and $\tilde{\gamma}$, we have $-16\tilde{\beta} + 4\tilde{\gamma}^2 + 4\tilde{\gamma} + 1 = 0$, and thus $\lambda_2 = \lambda_3 = \frac{4\tilde{\beta} - 2\tilde{\gamma} - 1}{4\tilde{\beta}}$ and $\lim_{\tilde{\omega} \to \infty} \rho(\mathbf{A}) = |\lambda_2| = \frac{1 - |\tilde{\alpha}|^2}{(1 + |\tilde{\alpha}|)^2}$, for $\tilde{\alpha} \in [-\frac{1}{3}, \frac{1}{3}]$.

3.3 TR-BDF2 scheme

In recent years, more and more research has been achieved on schemes with multiple sub-steps. Among them, we have several popular ones such as the TR-BDF2 scheme [3, 4, 47, 61] (also known as the Bathe scheme in some contexts). This scheme is a predictor-corrector scheme that uses the implicit trapezoidal rule (Crank-Nicolson) for the first sub-step by taking $\tilde{\gamma}\Delta t$ as the step and the second-order backward differentiation formula for the second one, using the data at t^n and calculated previously for the first sub-step.

$$\begin{cases} \operatorname{Seek} \mathbf{u}^{h,n+1}, \dot{\mathbf{u}}^{h,n+1}, \ddot{\mathbf{u}}^{h,n+1} \in \mathbf{V}^{h} \text{ s.t.} \\ \dot{\tilde{\mathbf{u}}}^{h,n+\tilde{\gamma}} = \dot{\mathbf{u}}^{h,n} + \frac{\tilde{\gamma}\Delta t}{2} \left(\ddot{\mathbf{u}}^{h,n} + \tilde{\mathbf{u}}^{h,n+\tilde{\gamma}} \right), & \text{(i)} \\ \ddot{\mathbf{u}}^{h,n+\tilde{\gamma}} = \mathbf{u}^{h,n} + \tilde{\gamma}\Delta t \mathbf{v}^{h,n} + \frac{\tilde{\gamma}^{2}\Delta t^{2}}{4} \left(\ddot{\mathbf{u}}^{h,n} + \tilde{\mathbf{u}}^{h,n+\tilde{\gamma}} \right), & \text{(ii)} \\ \mathbf{M}\ddot{\tilde{\mathbf{u}}}^{h,n+\tilde{\gamma}} + \mathbf{B}(\tilde{\mathbf{u}}^{h,n+\tilde{\gamma}}) = \mathbf{L}^{n+\tilde{\gamma}}, & \text{(iii)} \\ \dot{\mathbf{u}}^{h,n+1} = \frac{1}{\tilde{\gamma}(2-\tilde{\gamma})} \ddot{\mathbf{u}}^{h,n+\tilde{\gamma}} - \frac{(1-\tilde{\gamma})^{2}}{\tilde{\gamma}(2-\tilde{\gamma})} \dot{\mathbf{u}}^{h,n} + \frac{1-\tilde{\gamma}}{2-\tilde{\gamma}} \Delta t \ddot{\mathbf{u}}^{h,n+1}, & \text{(iv)} \\ \mathbf{u}^{h,n+1} = \frac{1}{\tilde{\gamma}(2-\tilde{\gamma})} \tilde{\mathbf{u}}^{h,n+\tilde{\gamma}} - \frac{(1-\tilde{\gamma})^{2}}{\tilde{\gamma}(2-\tilde{\gamma})} \mathbf{u}^{h,n} + \frac{1-\tilde{\gamma}}{2-\tilde{\gamma}} \Delta t \dot{\mathbf{u}}^{h,n+1}, & \text{(v)} \\ \mathbf{M}\ddot{\mathbf{u}}^{h,n+1} + \mathbf{B}(\mathbf{u}^{h,n+1}) = \mathbf{L}^{n+1}. & \text{(vi)} \end{cases}$$

A popular value for the parameter $\tilde{\gamma}$ can be taken as $2-\sqrt{2}$, in which case, the linear systems at the two sub-steps are identical for linear elasticity. This scheme is also dissipative. We define the amplification matrix and its spectral radius similarly and illustrate in Fig. 4 for $\tilde{\gamma}=2-\sqrt{2}$. This scheme is highly dissipative compared to the HHT- α scheme on high frequencies. Its spectral radius tends to zero when $\tilde{\omega}$ tends to $+\infty$ and this confirms an L-stability.

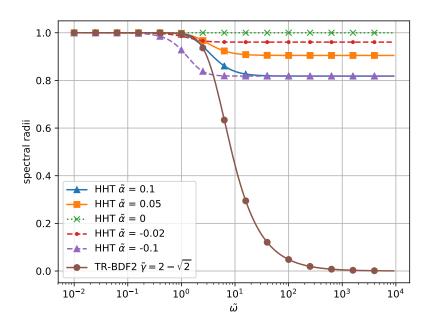


Figure 4: Spectral radii for HHT- α and TR-BDF2 schemes.

4 Numerical simulations

In this section, the numerical results for three different benchmarks (two uni-dimensional elastic problems and the bounce of a sphere) involving unilateral contact with a rigid obstacle are illustrated. In each simulation, the discrete modified energy will be displayed. For the two 1D tests, Nitsche's and penalty methods are combined with HHT- α and TR-BDF2 schemes. For the last test, Nitsche's and ALM are combined with HHT- α and TR-BDF2 schemes, and the hybrid Nitsche scheme [22] has also been applied. The nonlinear equations for each scheme (24)-(iii), (33)-(iii) and (vi) are solved by the semi-smooth Newton's method [69]. Moreover, the standard mass and mass redistribution methods are also compared. All numerical simulations are realized via finite element software GetFEM [70] using the Python interface.

An initial acceleration field has to be computed from the initial displacement and velocity fields, with $\ddot{\mathbf{u}}^0 = \mathbf{M}^{-1} \left(\mathbf{L}^0 - \mathbf{B}(\mathbf{u}^0) \right)$. It should be noted that with the mass redistribution method, the mass matrix \mathbf{M}^r is non-invertible (contrary to the normal mass matrix). Then, this is no longer possible to evaluate the initial acceleration with the previous formula. In our work, the initial acceleration field is calculated with the normal mass matrix, and during the numerical simulation, the velocity and acceleration on Γ_C are calculated by a backward formula and not the standard scheme, see e.g. Alg. 1 for the HHT- α scheme.

Remark. Without the reconstruction of the velocity and acceleration of DoFs on Γ_C , this is

Algorithm 1 One time-step using mass redistribution method with HHT- α scheme.

still possible to obtain results but the velocity and acceleration on Γ_C present often important additional oscillations (influenced by the initial truncation error and potential non-compatibility of the initial acceleration with initial displacement and velocity).

4.1 1D elastic bar with Signorini and Dirichlet boundary conditions

In this section, we consider the test case proposed in [28, Sect. 5] and named 1D-SD in what follows. The 1D bar is the solution to the following dynamic equilibrium problem:

Seek
$$u(x,t): [0,1] \times (0,T) \to \mathbb{R}$$
 s.t.
$$\begin{cases} \frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} = 0, \\ u(1,t) = 0, \\ u(0,t) \ge 0, \frac{\partial u}{\partial x}(0,t) \le 0, u(0,t) \frac{\partial u}{\partial x}(0,t) = 0, \\ u(x,0) = \frac{1}{2} - \frac{x}{2}, \frac{\partial u}{\partial t}(x,0) = 0. \end{cases}$$
(34)

The deformation of the bar at different times is illustrated in Fig. 5. Both a constant mesh size h=0.05 and time step $\Delta t=0.05$ are used. The Nitsche's parameter γ_0 and the penalty parameter ϵ_0 are chosen to be identical $\gamma_0=\frac{1}{\epsilon_0}=5$.

4.1.1 Crank-Nicolson scheme ($\tilde{\alpha} = 0$)

Firstly, the Crank-Nicolson scheme (HHT- α method with $\tilde{\alpha}=0$) is used and is considered as a referral scheme to study the effect of numerical dissipation. The numerical and analytical solutions are displayed in Fig. 6. From up to down, the displacement and the velocity at the contact point (x=0), the contact pressure, and the numerical energy are plotted. As expected, there is more penetration on Γ_C for the penalty method than for Nitsche's method since it is

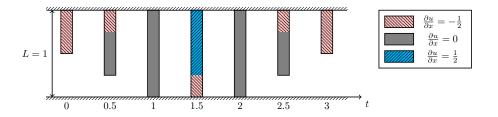


Figure 5: 1D-SD: Deformation of the bar at different times.

a non-consistent method, see Fig. 7. The average displacements at x=0 for the first contact period of Nitsche's and the penalty method, are 5.0×10^{-4} and -3.8×10^{-3} respectively. Stronger oscillations are observed with the standard mass method and the contact pressure varies around zero rather than remaining precisely at zero when the bar is not in contact with the obstacle, due to the linear Lagrange elements and the discontinuity on time of the contact pressure. The redistributed mass allows smoother solutions especially on contact pressure compared to the normal mass. We should also note that the numerical energy shown is the modified energy and the discrete mechanical energy is noisier at each contact (which is not shown in this paper), as the contact methods applied in this work are equipped with conserving-form energy and its evolution of energy is also bounded.

4.1.2 HHT- α scheme

The results for the HHT- α scheme with parameter $\tilde{\alpha} \in \{0.05, -0.02\}$ are illustrated in Fig. 8. A non-zero $\tilde{\alpha}$ helps to dissipate high-frequency oscillations as described in Sect. 3.1. More regular displacements are observed compared with those obtained with the Crank-Nicolson scheme. With the redistributed mass, the contact pressure maintains zero during non-contact phases. For a negative value $\tilde{\alpha} = -0.02$, as the dissipation starts at a lower frequency, we obtain a more regular solution but with more energy loss. The energy loss can be important with a negative but with a higher magnitude value of $\tilde{\alpha}$, so its value should be chosen cautiously in order to guarantee the reliability of numerical results. The value, for instance, $\tilde{\alpha} = -0.02$ provides a compromise between energy dissipation and oscillations.

4.1.3 TR-BDF2 scheme

The plots for TR-BDF2 scheme with $\tilde{\gamma}=2-\sqrt{2}$ are shown in Fig. 9. Fewer oscillations and energy dissipation are observed for TR-BDF2 than for HHT- α . The corrector sub-step helps to reduce the oscillation of velocity.

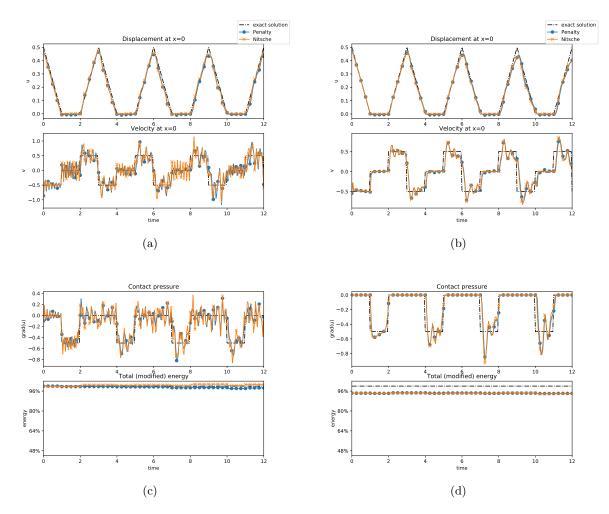


Figure 6: 1D-SD: Comparison of the analytical solution and the numerical solutions for standard (left) and modified (right) mass matrices with the Crank-Nicolson scheme ($\tilde{\alpha} = 0$).

4.1.4 Numerical convergence

In this test of convergence, various mesh sizes and time steps are applied by fixing the ratio $\frac{\Delta t}{h} = 1$, and the Nitsche's method has been used to enforce the Signorini's condition. The errors on $L^2(0,T;H^1(\Omega))$ -norm are illustrated in Fig. 10. A similar convergence order is observed for the HHT- α scheme with different values of parameter $\tilde{\alpha}$.

4.2 1D elastic bar with two Signorini boundary conditions

We propose here a new benchmark with an analytical solution: a 1D elastic bar with two rigid obstacles (at x = 0 and at x = 1.5) and is called 1D-SS in what follows. The bar is initially

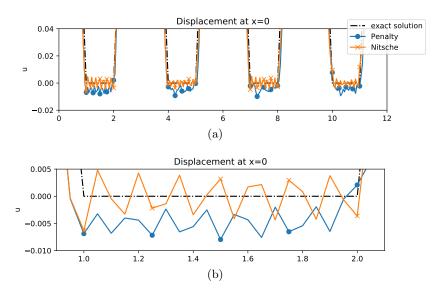


Figure 7: 1D-SD: Comparison of penalty and Nitsche methods on the penetration at x = 0 with the Crank-Nicolson scheme ($\tilde{\alpha} = 0$). The first contact period is zoomed in (b).

compressed to half-high and has a constant velocity $v_0 = -\frac{1}{2}$. The benchmark consists to solve the problem (35):

$$\begin{cases} \operatorname{Seek} \ u(x,t) : [0,1] \times (0,T) \to \mathbb{R}, \ \text{s.t.} \\ \frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} = 0, \\ u(0,t) \ge 0, \ \frac{\partial u}{\partial x}(0,t) \le 0, \ u(0,t) \frac{\partial u}{\partial x}(0,t) = 0, \\ u(1,t) \le \frac{1}{2}, \ \frac{\partial u}{\partial x}(1,t) \le 0, \ \left(u(1,t) - \frac{1}{2}\right) \frac{\partial u}{\partial x}(1,t) = 0, \\ u(x,0) = 1 - \frac{x}{2}, \ \frac{\partial u}{\partial t}(x,0) = -\frac{1}{2}. \end{cases}$$
(35)

The analytical solution is piecewise regular and periodic. The movement of the elastic bar (displaced position over time) is shown in Fig. 11 and the analytical solution is illustrated on the x-t diagram in Fig. 12. The impact of each side has three different states: 1. non-contact; 2. contact with a zero contact pressure; 3. contact with a contact pressure non-zero. The most interesting part of the benchmark is located at state 2, contact with a zero contact pressure state, e.g. for the side x=0 when $t \in [1,2]$. As mentioned in [23], the situation called "grazing contact" (both $u_n=0$ and $\frac{\partial u}{\partial x}=0$ on Γ_C) is a non-differentiable case for operators \mathbf{B}_N and \mathbf{B}_A .

The same combination of contact methods and time schemes as for Sect. 4.1 is used; and with the following parameters: mesh size h=0.05, the time step $\Delta t=0.05$, and $\gamma_0=\frac{1}{\epsilon_0}=5$. The mass redistribution method implies here that the mass is eliminated at both sides of the

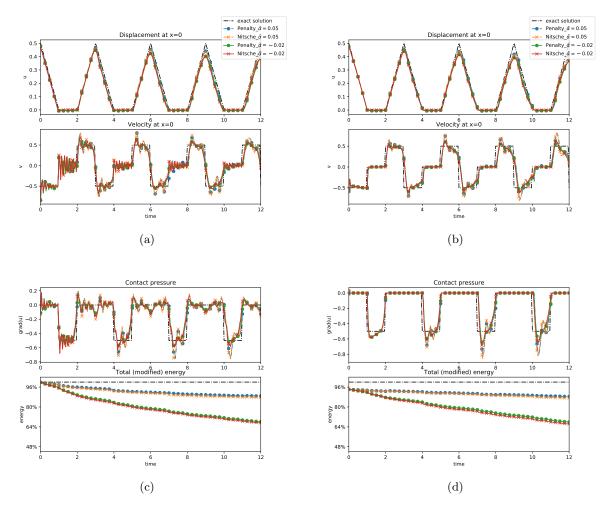


Figure 8: 1D-SD: Comparison of the analytical and discrete solutions for the standard (left) and modified (right) mass matrices with HHT- α method and $\tilde{\alpha} \in \{0.05, -0.02\}$.

bar.

4.2.1 Crank-Nicolson scheme ($\tilde{\alpha} = 0$)

The results obtained for the Crank-Nicolson scheme are shown in Fig. 13. Oscillations can be observed since the method is non-dissipative with the standard mass method. As with the modified mass method, the displacement and contact pressure are smoother, as expected. As this new benchmark contains no Dirichlet boundary condition, the whole system is on a free vibration coupled with contact on two sides, which makes the benchmark more complicated for numerical simulation.

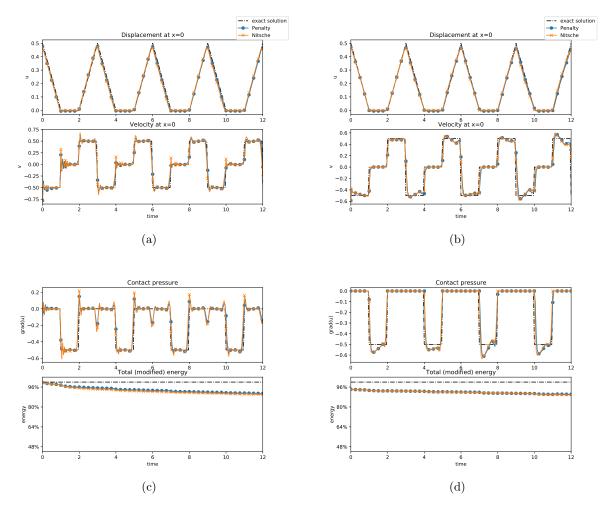


Figure 9: 1D-SD: Comparison of the analytical solution and discrete solutions for standard (left) and modified (right) mass matrices with TRBDF2 scheme.

4.2.2 HHT- α scheme

The numerical results for the HHT- α scheme with $\tilde{\alpha} \in \{0.05, -0.02\}$ are shown in Fig. 14. As expected, dissipation at high frequencies is observed. Moreover, as before, less oscillation is present for $\tilde{\alpha} = -0.02$ than for $\tilde{\alpha} = 0.05$ but the dissipation is higher. Once again, this value gives an interesting compromise between oscillation and energy dissipation; especially with the modified mass method.

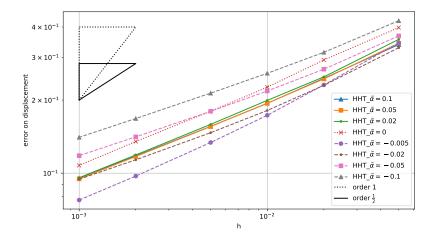


Figure 10: L^2H^1 -error vs h with $\frac{\Delta t}{h} = 1$.

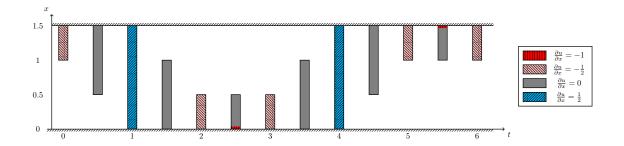


Figure 11: 1D-SS: "Wriggle" between two rigid obstacles.

4.2.3 TR-BDF2 scheme

The TR-BDF2 scheme is used with $\tilde{\gamma}=2-\sqrt{2}$ in Fig. 15. As expected, the results are better with this 2-step predictor-corrector scheme compared to the HHT- α scheme. As before, the modified mass method has less oscillation than the standard one.

4.3 3D impact of a sphere

The last benchmark is a three-dimensional sphere which impacts a rigid foundation at z=0. The center of the sphere is initially at $[0,0,2]^T$ with zero initial velocity and has a diameter D=40. The mesh used is a second-order tetrahedron mesh with h=4 and a constant time step is used. For a soft version, the Lamé coefficients are $\lambda=\mu=20$, and $\Delta t=0.25$; and for a hard version, the Lamé coefficients are $\lambda=\mu=30000$, and $\Delta t=0.05$. In both cases, the mass density

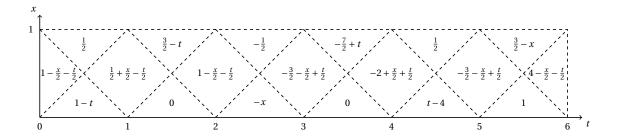


Figure 12: 1D-SS: Displacement in each region of the x-t diagram.

 $\rho=1$, and the gravity load is $\mathbf{f}=[0,0,-0.1]^T$. The lower part of the sphere is assigned with Signorini boundary conditions and on the upper part, a Neumann condition $\mathbf{f}_N=\mathbf{0}$ is applied. For the numerical simulation, quadratic Lagrange finite elements are used for the displacement and linear finite elements contact multiplier (when using the ALM). Moreover, in addition to HHT- α and TR-BDF2 schemes, the hybrid Nitsche scheme, which is introduced in Sect. A.3, is also tested here. The Nitsche's parameter γ_0 , the penalty parameter ϵ_0 , and the parameter γ_a for ALM are chosen to be identical $\gamma_0=\frac{1}{\epsilon_0}=\gamma_a=100\mu$. The deformed configuration with von Mises stress and contact pressure are displayed in Fig. 18. The deformation and the contact surface are more limited for the hard sphere as expected.

In Fig. 16 and Fig. 17, the results for the soft and hard spheres are illustrated respectively for both Nitsche's method and ALM. The HHT- α and the TR-BDF2 schemes produce a relatively smooth solution. As expected, the TR-BDF2 scheme provides smoother results for a comparable loss of energy than the HHT- α scheme. It is also noticed that the hybrid Nitsche scheme conserves very well the total modified energy as predicted by theory [22]. The hybrid Nitsche scheme behaves similarly to the mid-point scheme. This property ensures a strict conservation of energy during contact-free phases but at the same time spreads all high-frequency oscillations without damping. So the hybrid Nitsche scheme suffers from strong oscillations for the velocity field (see, e.g., Fig. 16b and 17b) comparing to the TR-BDF2 scheme which is dissipating. Note that numerical energy loss may still occur during transitions between contact and non-contact (see, e.g., Fig. 17).

4.3.1 Numerical cost

In this work, we focus on the implicit schemes so that the main numerical cost is due to the solving of non-linear equations by a Newton method. We display the absolute and relative CPU times in Tab. 1 evaluated sequentially on a computer equipped with an Intel[®] Core[™] i7-9850H CPU (Crank-Nicolson scheme with Nitsche's method are used as reference). We also display the number of Newton iterations on each time-step for different schemes in Fig. 19a with hybrid Nitsche scheme and in Fig. 19b without it in order to compare more closely the HHT- α and TR-BDF2 schemes (this is the sum of iterations of sub-steps for TR-BDF2 scheme). During

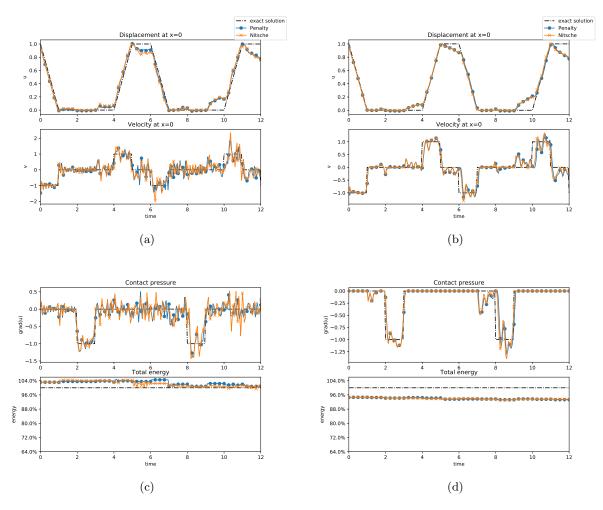


Figure 13: 1D-SS: Comparison of the analytical and discrete solutions for standard (left) and modified (right) mass matrices with the Crank-Nicolson method.

the non-contact (linear) regime, all schemes converge in two iterations (except for the TR-BDF2 scheme which takes four iterations since each sub-step needs two iterations). Generally, during contact phases, HHT- α and Crank-Nicolson schemes need four iterations (with a maximum of five iterations) and TR-BDF2 needs six iterations (with a maximum of eight iterations). However, the hybrid Nitsche scheme needs more than 25 iterations before convergence. The results of CPU time consumption are correlated to the number of Newton iterations.

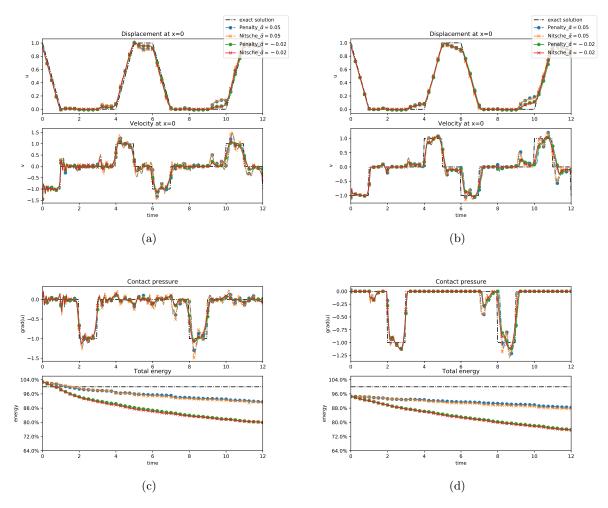


Figure 14: 1D-SS: Comparison of the analytical and discrete solutions for standard (left) and modified (right) mass matrices with HHT- α method and $\tilde{\alpha} \in \{0.05, -0.02\}$.

5 Conclusion

In this paper, we have applied HHT- α and TR-BDF2 schemes combined with the Nitsche's, penalty, and ALM methods. The comparative analysis was informed by three numerical simulation benchmarks. Our findings reveal the following insights:

- Notably, Nitsche's and ALM methods emerge as more compliant with contact conditions due to their intrinsic consistency. Conversely, the penalty method, while easier to implement, exhibits limitations in this regard.
- According to the simulation results, the TR-BDF2 scheme provides an interesting com-

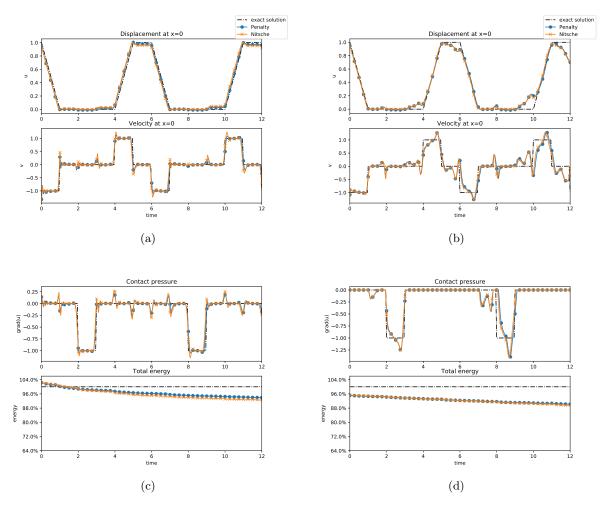


Figure 15: 1D-SS: Comparison of the analytical and discrete solutions for standard (left) and modified (right) mass matrices with TRBDF2 scheme.

promise between loss of energy and spurious oscillations but is more costly than HHT- α schemes. However, in some particular cases as for very fine time-steps, HHT- α can be more interesting since it is cheaper and dissipates less high frequencies.

- Compared to the others, the hybrid Nitsche scheme is more expensive and presents strong oscillations of the velocity. Furthermore, it is noteworthy that the hybrid Nitsche scheme exhibits the property of conserving energy in the linear regime, which might prove beneficial in specific scenarios.
- The mass redistribution method can also help to improve the performance [22] and provides more accurate contact pressure.

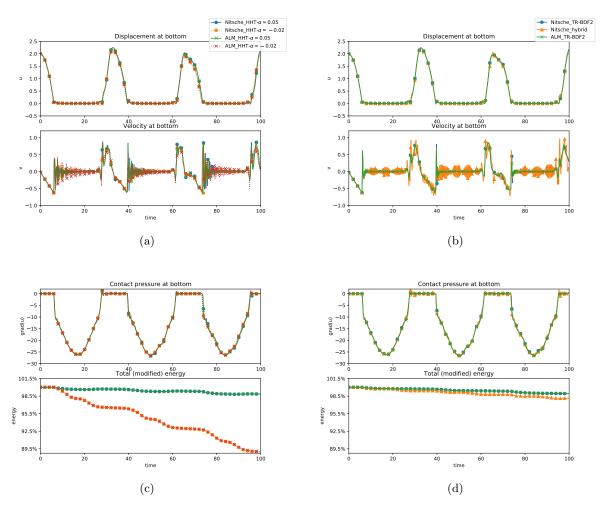


Figure 16: 3D impact of a soft sphere: Discrete solution for HHT- α (left), TR-BDF2 and Nitschehybrid (right) schemes.

		Nitsche's method		ALM	
Crank-Nicolson	CPU time (s) & Ratio	461.4475	1	488.3083	1.0582
	Total iterations & Ratio	1129	1	1181	1.0461
HHT- α ($\tilde{\alpha} = 0.05$)	CPU time (s) & Ratio	472.2333	1.0234	472.4737	1.0239
	Total iterations & Ratio	1121	0.9929	1111	0.9841
TR-BDF2	CPU time (s) & Ratio	840.3112	1.8210	842.9750	1.8268
	Total iterations & Ratio	2079	1.8415	2076	1.8388
hybrid Nitsche	CPU time (s) & Ratio	3541.2730	7.6743	Not concerned	Not concerned
	Total iterations & Ratio	7452	6.6005	Not concerned	Not concerned

Table 1: 3D impact of a sphere: Numerical cost for different methods (with Nitsche's method and Crank-Nicolson scheme as reference).

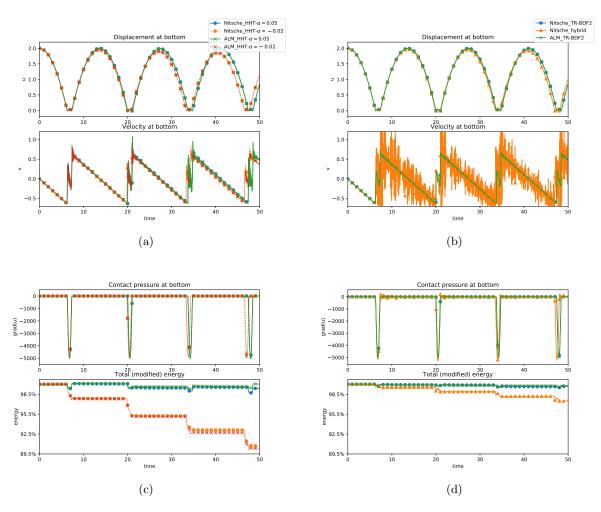


Figure 17: 3D impact of a hard sphere: Discrete solution for HHT- α (left), TR-BDF2 and Nitsche-hybrid (right) schemes.

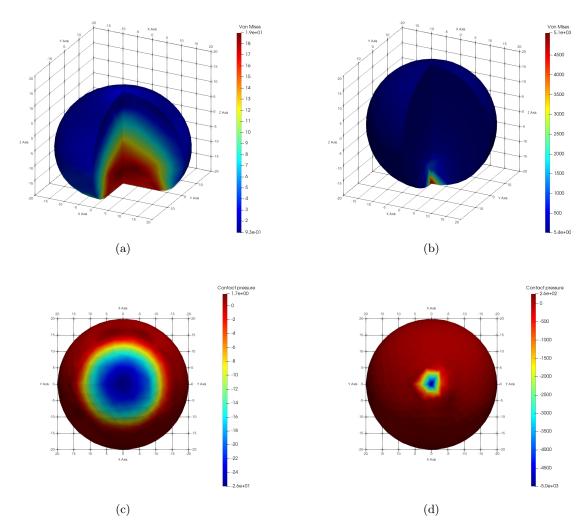


Figure 18: 3D impact of a sphere: deformed configuration with von Mises stress (up), and contact pressure (down) for the soft sphere at t=16 (left) and the hard sphere at t=6.8 (right), for Nitsche's method with HHT- α scheme ($\tilde{\alpha}=0.05$).

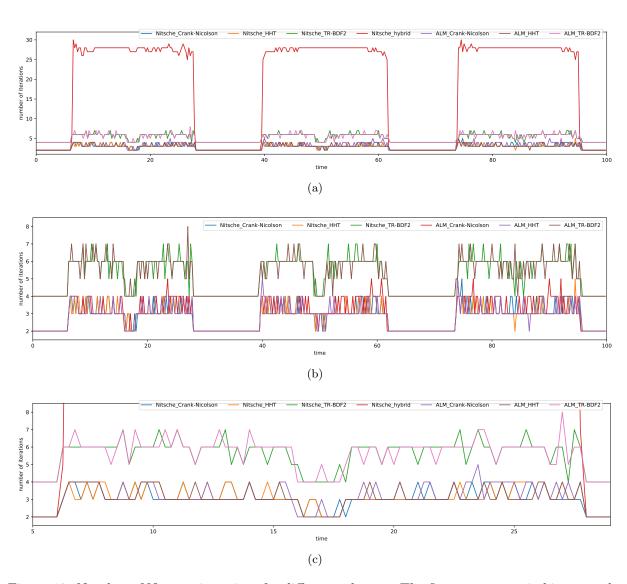


Figure 19: Number of Newton iterations for different schemes. The first contact period is zoomed on (c).

We would also like to note that the numerical results realized with Nitsche's method and skew-symmetric or non-symmetric versions, or other formulations of ALM are feasible but they are not shown here since we limit ourselves to variants that conserve a modified energy. In fact, the skew-symmetric version of Nitsche's method can be even more robust for a few simulations.

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A Appendices

The first appendix details the local truncation error for the HHT-alpha scheme. The second appendix provides the complete amplification matrix for HHT-alpha. The third one provides an introduction to the Nitsche-Hybrid scheme.

A.1 Local truncation error for HHT- α scheme

Applying the local truncation error (27) to the SDOF system (25), the following holds:

$$\Delta t T_{n} = \frac{-\tilde{\alpha}\omega^{2}\Delta t^{2} + \frac{1}{\tilde{\beta}}}{\omega^{2}\Delta t^{2} (1 - \tilde{\alpha}) + \frac{1}{\tilde{\beta}}} u(t^{n}) + \frac{\frac{1}{\tilde{\beta}}}{\omega^{2}\Delta t^{2} (1 - \tilde{\alpha}) + \frac{1}{\tilde{\beta}}} \Delta t \dot{u}(t^{n})$$

$$+ \frac{1 - 2\tilde{\beta}}{2\tilde{\beta} \left(\omega^{2}\Delta t^{2} (1 - \tilde{\alpha}) + \frac{1}{\tilde{\beta}}\right)} \Delta t^{2} \ddot{u}(t^{n}) - u(t^{n}) - \Delta t \dot{u}(t^{n}) - \frac{1}{2}\Delta t^{2} \ddot{u}(t^{n}) + O(\Delta t^{3})$$

$$= \frac{-\omega^{2}\Delta t^{2}}{\omega^{2}\Delta t^{2} (1 - \tilde{\alpha}) + \frac{1}{\tilde{\beta}}} u(t^{n}) + \frac{(1 - \tilde{\alpha})\omega^{2}\Delta t^{2}}{\omega^{2}\Delta t^{2} (1 - \tilde{\alpha}) + \frac{1}{\tilde{\beta}}} \Delta t \dot{u}(t^{n})$$

$$+ \frac{1}{2} \left(\frac{(1 - 2\tilde{\beta})\frac{1}{\tilde{\beta}}}{\omega^{2}\Delta t^{2} (1 - \tilde{\alpha}) + \frac{1}{\tilde{\beta}}} - 1\right) \Delta t^{2} \ddot{u}(t^{n}) + O(\Delta t^{3}),$$

$$= \frac{1}{\omega^{2}\Delta t^{2} (1 - \tilde{\alpha}) + \frac{1}{\tilde{\beta}}} \left(-\omega^{2}\Delta t^{2} u(t^{n}) - \left(1 + \frac{\omega^{2}\Delta t^{2} (1 - \tilde{\alpha})}{2}\right) \Delta t^{2} \ddot{u}(t^{n})\right)$$

$$+ \frac{(1 - \tilde{\alpha})\omega^{2}\Delta t^{2}}{\omega^{2}\Delta t^{2} (1 - \tilde{\alpha}) + \frac{1}{\tilde{\beta}}} \Delta t \dot{u}(t^{n}) + O(\Delta t^{3})$$

$$= \frac{1}{\omega^{2}\Delta t^{2} (1 - \tilde{\alpha}) + \frac{1}{\tilde{\beta}}} \left(-\left(\omega^{2}u(t^{n}) + \ddot{u}(t^{n})\right) \Delta t^{2} - \frac{\omega^{2}\Delta t^{2} (1 - \tilde{\alpha})}{2} \Delta t^{4} \ddot{u}(t^{n})\right)$$

$$+ \frac{(1 - \tilde{\alpha})\omega^{2}}{\omega^{2}\Delta t^{2} (1 - \tilde{\alpha}) + \frac{1}{\tilde{\beta}}} \Delta t^{3} \dot{u}(t^{n}) + O(\Delta t^{3})$$

$$\leq \frac{1}{\omega^{2}\Delta t^{2} (1 - \tilde{\alpha}) + \frac{1}{\tilde{\beta}}} |\omega^{2}u(t^{n}) + \ddot{u}(t^{n})| \Delta t^{2} + \frac{(1 - \tilde{\alpha})\omega^{2}}{\omega^{2}\Delta t^{2} (1 - \tilde{\alpha}) + \frac{1}{\tilde{\beta}}} |\dot{u}(t^{n})| \Delta t^{3} + O(\Delta t^{3}),$$
(36)

which implies the boundness of the local truncation error.

A.2 Amplification matrix for HHT- α scheme

Applying the HHT- α scheme (24) to the SDOF system (25), by replacing the operators **M** and **B** by m and k respectively, the amplification matrix for the HHT- α scheme reads below:

$$\begin{bmatrix} \frac{-\tilde{\alpha}\tilde{\omega}^{2} + \frac{1}{\tilde{\beta}}}{\tilde{\omega}^{2}(1-\tilde{\alpha}) + \frac{1}{\tilde{\beta}}} & \frac{1}{\tilde{\beta}\left(\tilde{\omega}^{2}(1-\tilde{\alpha}) + \frac{1}{\tilde{\beta}}\right)} & \frac{1-2\tilde{\beta}}{2\tilde{\beta}\left(\tilde{\omega}^{2}(1-\tilde{\alpha}) + \frac{1}{\tilde{\beta}}\right)} \\ \tilde{\gamma}\left(\frac{-\tilde{\alpha}\tilde{\omega}^{2} + \frac{1}{\tilde{\beta}}}{\tilde{\beta}\left(\tilde{\omega}^{2}(1-\tilde{\alpha}) + \frac{1}{\tilde{\beta}}\right)} - \frac{1}{\tilde{\beta}}\right) & \tilde{\gamma}\left(-\frac{1}{\tilde{\beta}} + \frac{1}{\tilde{\beta}^{2}\left(\tilde{\omega}^{2}(1-\tilde{\alpha}) + \frac{1}{\tilde{\beta}}\right)}\right) + 1 & \tilde{\gamma}\left(\frac{2\tilde{\beta} - 1}{2\tilde{\beta}} + \frac{1-2\tilde{\beta}}{2\tilde{\beta}^{2}\left(\tilde{\omega}^{2}(1-\tilde{\alpha}) + \frac{1}{\tilde{\beta}}\right)}\right) - \tilde{\gamma} + 1 \\ \frac{-\tilde{\alpha}\tilde{\omega}^{2} + \frac{1}{\tilde{\beta}}}{\tilde{\beta}\left(\tilde{\omega}^{2}(1-\tilde{\alpha}) + \frac{1}{\tilde{\beta}}\right)} - \frac{1}{\tilde{\beta}} & -\frac{1}{\tilde{\beta}} + \frac{1}{\tilde{\beta}^{2}\left(\tilde{\omega}^{2}(1-\tilde{\alpha}) + \frac{1}{\tilde{\beta}}\right)} & \frac{2\tilde{\beta} - 1}{2\tilde{\beta}} + \frac{1-2\tilde{\beta}}{2\tilde{\beta}^{2}\left(\tilde{\omega}^{2}(1-\tilde{\alpha}) + \frac{1}{\tilde{\beta}}\right)} \\ \end{cases}$$

$$(37)$$

We recall that $\mathbf{Y}^{n+1} = \mathbf{A}\mathbf{Y}^n$ with $\mathbf{Y}^n = [u^n, \Delta t \dot{u}^n, \Delta t^2 \ddot{u}^n]^T$ and $\tilde{\omega} := \omega^2 \Delta t^2$.

A.3 Nitsche-Hybrid time scheme

The Nitsche-Hybrid scheme has been introduced in [22] and solved the following system at each time step:

$$\begin{cases}
\operatorname{Seek} \mathbf{u}^{h,n+1}, \dot{\mathbf{u}}^{h,n+1}, \ddot{\mathbf{u}}^{h,n+1} \in \mathbf{V}^{h} \text{ s.t.} \\
\mathbf{u}^{h,n+1} = \mathbf{u}^{h,n} + \frac{\Delta t}{2} (\dot{\mathbf{u}}^{h,n} + \dot{\mathbf{u}}^{h,n+1}), \\
\dot{\mathbf{u}}^{h,n+1} = \dot{\mathbf{u}}^{h,n} + \frac{\Delta t}{2} (\ddot{\mathbf{u}}^{h,n} + \ddot{\mathbf{u}}^{h,n+1}), \\
\frac{\mathbf{M}}{2} (\ddot{\mathbf{u}}^{h,n} + \ddot{\mathbf{u}}^{h,n+1}) + \mathbf{B}_{Nh} (\mathbf{u}^{h,n}, \mathbf{u}^{h,n+1}) = \frac{1}{2} (\mathbf{L}^{n} + \mathbf{L}^{n+1}).
\end{cases} (38)$$

where non-linear operator \mathbf{B}_{Nh} is defined by integration:

$$\begin{split} \left(\mathbf{B}_{Nh}(\mathbf{u}^{h,n},\mathbf{u}^{h,n+1}),\mathbf{w}^{h}\right)_{\Omega} = &\frac{1}{2}\left(a_{\gamma_{N}}(\mathbf{u}^{h,n},\mathbf{w}^{h}) + a_{\gamma_{N}}(\mathbf{u}^{h,n+1},\mathbf{w}^{h})\right) \\ &+ \left(\frac{1}{\gamma_{N}}H(P_{N}(\mathbf{u}^{h,n}))\left[\frac{1}{2}(P_{N}(\mathbf{u}^{h,n}+\mathbf{u}^{h,n+1}))\right]_{\mathbb{R}^{-}},\mathbf{w}^{h}\right)_{\Gamma_{C}} \\ &+ \left(\frac{1}{\gamma_{N}}H(-P_{N}(\mathbf{u}^{h,n}))\frac{1}{2}\left(\left[P_{N}(\mathbf{u}^{h,n})\right]_{\mathbb{R}^{-}} + \left[P_{N}(\mathbf{u}^{h,n+1})\right]_{\mathbb{R}^{-}}\right),\mathbf{w}^{h}\right)_{\Gamma_{C}}, \end{split}$$

$$(39)$$

where $H(\cdot)$ is the Heaviside function. This scheme is unconditionally stable for the symmetric version of Nitsche's method. The main idea is to combine two different schemes with one during contact phases and one during non-contact phases. Hence, this scheme conserves the mechanical energy on the linear regime (when the contact is not active) as its equivalence with the mid-point scheme but it dissipates during contact phases. Moreover, this scheme is more nonlinear than the others and a bit more difficult to implement.

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