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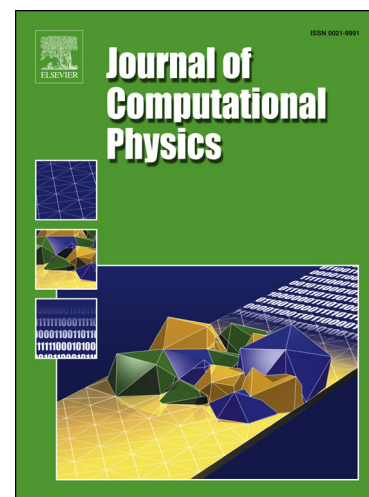
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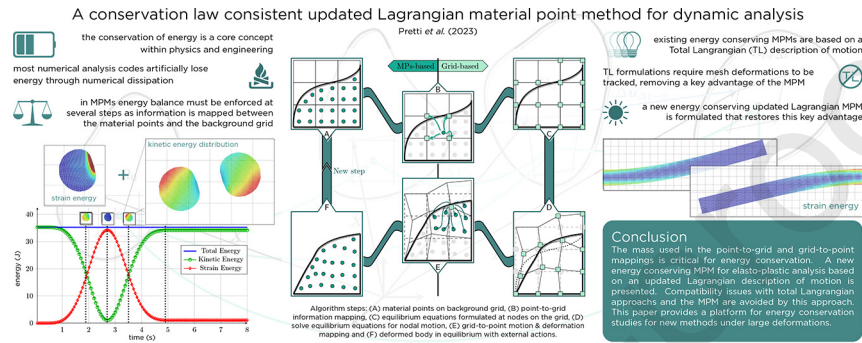
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## Graphical abstract

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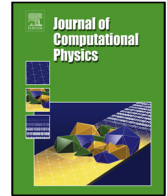
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**Highlights**

- First energy conserving, updated Lagrangian Material Point Method for solid dynamics.
- Energy and momenta losses in Material Point Methods are clarified and explained.
- Adaptive time-stepping technique is formulated based on the CFL condition.



# A conservation law consistent updated Lagrangian material point method for dynamic analysis

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## ABSTRACT

The Material Point Method (MPM) is well suited to modelling dynamic solid mechanics problems undergoing large deformations with non-linear, history dependent material behaviour. However, the vast majority of existing material point method implementations do not inherit conservation properties (momenta and energy) from their continuum formulations. This paper provides, for the first time, a dynamic updated Lagrangian material point method for elasto-plastic materials undergoing large deformation that guarantees momenta and energy conservation. Sources of energy dissipation during point-to-grid and grid-to-point mappings for FLuid Implicit Particle (FLIP) and Particle In Cell (PIC) approaches are clarified and a novel time-stepping approach is proposed based on an efficient approximation of the Courant-Friedrich-Lewy (CFL) condition. The formulation provided in this paper provides a platform for understanding the energy conservation nature of future/existing features of material point methods, such as contact approaches.

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## 1. Introduction

The Material Point Method for solids, (as originally described in [1–3]) is receiving significant interest for problems involving very large deformations, with particular interest in geotechnical engineering. Recent reviews of the literature can be found in a number of papers [4; 5]. Historically, the MPM for solid mechanics was derived from the FLIP (fluid-

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APIC: Affine Particle In Cell; CFL: Courant-Friedrich-Lewy; FEM: Finite Element Method; FLIP: FLuid Implicit Particle; GIMPM: Generalised Interpolation Material Point Method; MPM: Material Point Method; PIC: Particle In Cell; PolyPIC: POLYnomial Particle In Cell; TL: Total Lagrangian; UL: Updated Lagrangian; XPIC: eXtended Particle In Cell."

implicit-particle) method [6; 7] which in turn, was a particularisation of the PIC (particle-in-cell) [8–10] method<sup>1</sup>. The MPM works by decoupling the representation of the problem domain (using “material points”) with the calculation phase which is carried out on a finite element grid. Such a split requires mapping of information from material points to the grid prior to the calculation phase and then the other way following calculation. Momenta and energy conservation in the MPM remain a matter of concern with respect to these mappings, as evidenced by the numerous publications in this area: [6; 8; 11–14], among others.

Dynamic solid mechanics problems are often solved using an explicit approach to time discretisation, and this is the case with the majority of MPM research to date, see [15–17] although it should be noted that these publications are cast within small and not large deformation theory. Fewer researchers have used implicit time integration. Love’s and Sulsky’s 2006 papers [18; 19] provided theoretically sound bases for both the mapping procedures and the formulation of discrete equations, on the basis of the groundwork laid by several other publications (e.g. [20–25]). In particular, the constitutive relationship cast within finite deformation elasto-plasticity and the mid-point rule for the time integration scheme are discussed and assessed in the above-mentioned papers for the Finite Element Method.

If finite strain theory is taken into account, the difference between the current (or updated) and the initial (or total) Lagrangian reference frame is not negligible, making the frame used for the equilibrium equations a choice in terms of the numerical implementation of a method. For the MPM, the choice between an updated or a total (spatial or material) Lagrangian formulation is discussed in [26] which concludes that total Lagrangian formulations are not ideal for MPMs as they require the basis functions to be mapped back to the original coordinates, which is “*not practical as it would require mesh deformation throughout the analysis to be stored, destroying one of the key advantages of the material point method*” [26]. Therefore, while Love and Sulsky [18; 19] have provided an energy conserving total Lagrangian MPM here we overcome the limitations of a total approach via the derivation, implementation, verification and validation of a new updated Lagrangian energy conserving MPM for large deformation elasto-plastic dynamic analysis. It should be emphasised that, while Love and Sulsky [19] state their approach to be “updated Lagrangian”, their actual formulation is total Lagrangian, as can be seen from the adopted stress measure and integration volume used when satisfying the governing equations (see Coombs *et al.* [26] for a detailed discussion on the differences between total and updated Lagrangian formulations in the material point method). In addition to this key contribution of the paper, we also investigate the grid-to-point and point-to-grid mappings that are required in the MPM in terms of energy conservation. The conditions under which (linear and angular) momenta and energy are and are not conserved are clearly defined for PIC and FLIP motion projections within the MPM.

Section 2 of this paper presents the continuum and discretised equations for a deformable body in an UL and TL framework. Section 3 reviews the MPM computational cycle, focusing on its implicit version. In Sections 4 and 5, conservation properties are assessed. In particular, Section 4 examines conservation applied to the mappings (PIC and FLIP), while Section 5 develops an UL version of the energy-conserving internal force vector. Due to the well-

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<sup>1</sup>From this point on, the terms FLIP and PIC are used to define only the mapping procedures at the beginning and end of the step, and not the complete numerical methods.

recognised link between the implicit MPM and standard finite elements (see Guilkey and Weiss [27]), the discussion in Section 5 can also be applied to the Finite Element Method. Since selecting an adequate time-step length for dynamic MPM simulations is critical to complete any simulation, an adaptive time-step technique is introduced in Section 6. Finally, in Section 7, numerical examples demonstrating the conserving properties are shown for the bi-dimensional and three-dimensional cases. Section 8 concludes the paper with observations and possible future expansions of the current work.

## 2. Governing equations

In this section, the equations governing the continuum dynamics of a deformable body are briefly introduced. In particular, the balance of linear momentum is presented in different frames and in strong and weak forms. Hyperelastic-plastic constitutive models are considered with isotropic finite strain multiplicative plasticity (a *Hencky* material). In what follows, non-bold quantities represent scalars, while bold symbols indicate vectors or matrices. The use of index notation when necessary not only avoids confusion among these quantities, i.e., vectors and matrices, but also indicates their dimensions. In particular, uppercase letters in italic font ( $I, J, \dots$ ) indicate the degrees of freedom of the grid, uppercase upright letters ( $A, B, \dots$ ) denote grid nodal values, and lowercase letters ( $i, j, \alpha, \dots$ ) refer to the dimensions  $n^{dim}$  of the Euclidean space under consideration. In addition, the Einstein summation notation for subscript indexes is used throughout unless specified otherwise.

### 2.1. Notation, strong and weak forms

Consider a body  $\mathcal{B}$ , occupying an initial volume  $\Omega_0$  of the Euclidean three-dimensional space  $\mathcal{E} \subset \mathbb{R}^{n^{dim}}$ . The boundaries of the initial volume are  $\Gamma_0$ , partitioned into disjoint subsets such that  $\Gamma_0 = \Gamma_\varphi^0 \cup \Gamma_{\bar{\varphi}}^0$ , and  $\Gamma_\varphi^0 \cap \Gamma_{\bar{\varphi}}^0 = \emptyset$ . Particles constituting the volumes  $\Omega_0$  have a *reference density*  $\rho_0$  and occupy an *initial position*  $X$  in the initial reference frame. Let the same particles be denoted by  $\mathbf{x}$  in the current configuration  $\Omega$ , and let us introduce a smooth mapping  $\varphi$ , i.e., the *motion*, such that  $\varphi : \Omega_0 \times [0, T] \rightarrow \mathcal{E}$  and  $\mathbf{x} = \varphi(X, t)$ , with  $t \in [0, T] \subset \mathbb{R}$  being the time. Moreover, any motion  $\varphi$  belongs to the set of *admissible configurations*, defined as

$$\mathcal{K} = \{\varphi \mid \det(\mathbf{F}) > 0 \wedge \varphi = \bar{\varphi} \text{ on } \Gamma_{\bar{\varphi}}^0\}, \quad (1)$$

where  $\bar{\varphi}$  defines the *prescribed motions* on the boundary  $\Gamma_{\bar{\varphi}}^0$ , and  $\mathbf{F}$  indicates the *deformation gradient*, which is

$$F_{ij} := \frac{\partial \varphi_i}{\partial X_j} = \frac{\partial x_i}{\partial X_j}. \quad (2)$$

The *Jacobian*  $J$ , which is the determinant of the deformation gradient  $\mathbf{F}$ , can be used both to express the *current density*  $\rho = J^{-1} \rho_0$  and its infinitesimal *current volume*  $dV = J dV^0$ , with  $dV^0$  being the infinitesimal initial volume. We also introduce the difference between the reference and the current configuration of a particle, i.e., the *displacement*, as  $\mathbf{u}(X, t) = \mathbf{x} - X$ .

A point  $X$  has a *material velocity* defined as  $\mathbf{v} := \dot{\varphi}$ , where the notation  $(\bullet)$  indicates the material time derivative. Conventional stress measures are used: the *Cauchy* stress tensor  $\boldsymbol{\sigma}$ , the *Kirchhoff* stress tensor  $\boldsymbol{\tau}$  and the *first* and the

second Piola-Kirchhoff stress tensors  $\mathbf{P}$  and  $\mathbf{S}$ . The relationships between these quantities are

$$\boldsymbol{\sigma} = \mathbf{J}^{-1} \boldsymbol{\tau} = \mathbf{J}^{-1} \mathbf{P} \mathbf{F}^T = \mathbf{J}^{-1} \mathbf{F} \mathbf{S} \mathbf{F}^T, \quad (3)$$

where the superscript  $(\bullet)^T$  indicates the transpose of the quantity  $(\bullet)$ .

The local balance of momentum can be expressed in different frames. In the *updated* Lagrangian formulation, the equations are expressed in the current frame, leading the local balance of momentum to be

$$\frac{\partial \sigma_{ij}}{\partial x_j} + \rho (b_i - \dot{v}_i) = \mathbf{0}, \quad (4)$$

with  $(\rho \mathbf{b})$  being the *body forces*. In the *total* Lagrangian formulation, equations are based on the reference (or initial) frame, Eq. (4) becomes

$$\frac{\partial P_{ij}}{\partial X_j} + \rho_0 (b_i - \dot{v}_i) = \mathbf{0}. \quad (5)$$

Equations (4) and (5) are expressed in a strong form. The multiplication of the above equations by *weight functions*  $\boldsymbol{\eta}$ , belonging to the set of  $\mathcal{V} = \{\boldsymbol{\eta} \mid \boldsymbol{\eta} = \mathbf{0} \text{ on } \Gamma_\varphi^0\}$ , and the integration over the respective volumes permit the recasting of Eqs. (4) and (5) into the weak forms

$$\int_{\Omega} \sigma_{ij} \frac{\partial^{sym} \eta_i}{\partial x_j} dV - \int_{\Omega} \rho (b - \dot{v}_i) \eta_i dV - \int_{\Gamma_i} \bar{t}_i \eta_i dA = 0, \quad \forall \boldsymbol{\eta} \in \mathcal{V}; \quad (6)$$

$$\int_{\Omega_0} P_{ij} \frac{\partial \eta_i}{\partial X_j} dV_0 - \int_{\Omega_0} \rho_0 (b_i - \dot{v}_i) \eta_i dV_0 - \int_{\Gamma_i^0} \bar{t}_i^0 \eta_i dA_0 = 0, \quad \forall \boldsymbol{\eta} \in \mathcal{V}, \quad (7)$$

where a motion  $\boldsymbol{\varphi} \in \mathcal{K}$  and satisfying the initial conditions  $\boldsymbol{\varphi}(\mathbf{X}, 0) = \boldsymbol{\varphi}_0$  and  $\dot{\boldsymbol{\varphi}}(\mathbf{X}, 0) = \mathbf{v}_0$  has to be found. In the above equations,  $dA$  and  $dA_0$  represent the infinitesimal current and initial areas.

## 2.2. Space discretisation

Since the implicit MPM is closely related to the standard finite element method, we develop the discretised weak form firstly in the latter. Let an *isoparametric finite element Cartesian grid* discretise the continuum body  $\mathcal{B}$ , with  $N_{nodes}$  being the total number of nodes in the grid. The interpolated values of admissible motions and weight functions, belonging to the finite-dimensional sets  ${}^h\mathcal{K}$  and  ${}^h\mathcal{V}$ , are given by

$${}^h\varphi_i(\mathbf{x}) = \mathbf{N}_{il}(\mathbf{x}) \varphi_I; \quad (8)$$

$${}^h\eta_i(\mathbf{x}) = \mathbf{N}_{il}(\mathbf{x}) \eta_I; \quad (9)$$

$$\frac{\partial {}^h\eta_i}{\partial x_j}(\mathbf{x}) = \nabla_{x_j} \mathbf{N}_{il}(\mathbf{x}) \eta_I, \quad (10)$$

where index  $I = 1, \dots, (N_{nodes} \times n^{dim})$  represents the degrees of freedom of the whole discretisation, while  $\mathbf{N}(\mathbf{x})$  are the *shape functions*. Several options exist in the MPM for the shape functions as discussed in Sołowski *et al.* [5]. However, in this work, linear shape functions (MPM) or a convolution of linear shape functions with step characteristic functions (GIMPM) are considered in the examples in Section 7 (for a detailed explanation of this procedure, see

Bardenhagen and Kober [28]). The introduction of the grid allows Eqs. (6) and (7) to be written as

$$\int_{h\Omega} (\nabla_{x_j} N_{li}) \sigma_{ij} d^h V - \int_{h\Omega} \rho N_{li} (b_i - N_{iK} \dot{v}_K) d^h V - \int_{h\Gamma} N_{li} \bar{t}_i d^h A \approx \mathbf{0}; \quad (11)$$

$$\int_{h\Omega_0} (\nabla_{X_j} N_{li}) F_{ip} S_{pj} d^h V_0 - \int_{h\Omega_0} \rho_0 N_{li} (b_i - N_{iK} \dot{v}_K) d^h V_0 - \int_{h\Gamma_0} N_{li} \bar{t}_i^0 d^h A_0 \approx \mathbf{0}, \quad (12)$$

where the dependency of the quantities in the above equations from the current position  $\mathbf{x}$  or the displacement  $\mathbf{u}$  is dropped for the sake of clarity.

Let also the same body  $\mathcal{B}$  be described by a finite number of *material points*  $N_{pt}$ . In the original MPM [1], material points are used as quadrature points to approximate the above integrals. Furthermore, to allow compact presentation of Eqs. (11) and (12), the *internal force vectors*, the *consistent mass matrix* and the *external force vectors* are introduced along with their integral approximations

$$\mathbf{f}_I^{int} := \int_{h\Omega} (\nabla_{x_j} N_{li}) \sigma_{ij} \approx \sum_{pt} \nabla_{x_j} N_{li}(\mathbf{x}^{pt}) \sigma_{ij}(\mathbf{x}^{pt}) V^{pt}; \quad (13)$$

$$\mathbf{F}_I^{int} := \int_{h\Omega_0} (\nabla_{X_j} N_{li}) F_{ip} S_{pj} d^h V_0 \approx \sum_{pt} \nabla_{X_j} N_{li}(\mathbf{x}^{pt}) F_{ip}(\mathbf{x}^{pt}) S_{pj}(\mathbf{x}^{pt}) V_0^{pt}; \quad (14)$$

$$\mathbf{M}_{IK} := \int_{h\Omega} \rho N_{li} N_{iK} d^h V = \int_{h\Omega_0} \rho_0 N_{li} N_{iK} d^h V_0 \approx \sum_{pt} m^{pt} N_{li}(\mathbf{x}^{pt}) N_{iK}(\mathbf{x}^{pt}); \quad (15)$$

$$\mathbf{f}_I^{ext} := \int_{h\Omega} \rho N_{li} b_i d^h V + \int_{h\Gamma} N_{li} \bar{t}_i d^h A \approx \sum_{pt} m^{pt} N_{li}(\mathbf{x}^{pt}) b_i + \int_{h\Gamma} N_{li} \bar{t}_i d^h A; \quad (16)$$

$$\mathbf{F}_I^{ext} := \int_{h\Omega_0} \rho_0 N_{li} b_i d^h V_0 + \int_{h\Gamma_0} N_{li} \bar{t}_i^0 d^h A_0 \approx \sum_{pt} m^{pt} N_{li}(\mathbf{x}^{pt}) b_i + \int_{h\Gamma_0} N_{li} \bar{t}_i^0 d^h A_0, \quad (17)$$

where the superscript  $(\bullet)^{pt}$  implies that the quantity  $(\bullet)$  is computed at the material point location.

Since the *lumped* mass matrix  $\bar{\mathbf{M}}$  is often used in place of a consistent mass matrix and evaluating the conservation properties for both of the cases is one of the scopes of this work, it is useful to introduce the *effective* mass matrix  $\tilde{\mathbf{M}}$  as a linear combination of the two. In this way, they can be both generically expressed as

$$\tilde{\mathbf{M}} := (1 - \epsilon) \mathbf{M} + \epsilon \bar{\mathbf{M}} \quad \text{with} \quad \epsilon = [0, 1], \quad (18)$$

having introduced the lumped mass matrix defined as follows

$$\bar{\mathbf{M}}_{IK} := \delta_{IK} \int_{h\Omega} \rho N_K d^h V \approx \delta_{IK} \sum_{pt=1}^{N_{pt}} m^{pt} N_K(\mathbf{x}^{pt}) \quad (\text{no summation over } K). \quad (19)$$

Thus, the approximated compact forms of Eqs. (11) and (12) are

$$\mathbf{r}_I(\mathbf{u}) = \mathbf{f}_I^{int} + \tilde{\mathbf{M}}_{IK} \dot{v}_K - \mathbf{f}_I^{ext} \approx \mathbf{0}; \quad (20)$$

$$\mathbf{R}_I(\mathbf{u}) = \mathbf{F}_I^{int} + \tilde{\mathbf{M}}_{IK} \dot{v}_K - \mathbf{F}_I^{ext} \approx \mathbf{0}. \quad (21)$$

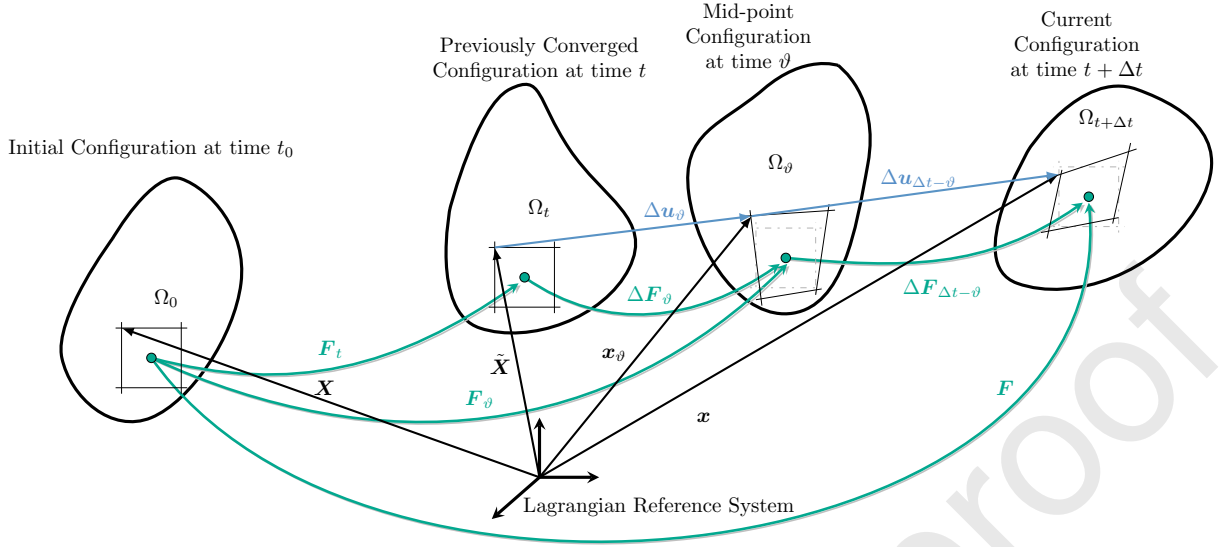


Fig. 1: Configurations taken into account by the current MPM formulation and associated quantities: grid positions, grid (incremental) displacements, material point deformation gradients.

### 2.3. Time discretisation

In a dynamic problem, the temporal problem duration  $[0, T]$  is discretised into steps of length  $\Delta t$ . Following Simo and Tarnow [20] for the FE method and Love and Sulsky for the MPM [19], we use the implicit *mid-point rule* since its use preserves angular momentum during the time-step when finite strain theory is considered<sup>2</sup>. Thus, the configuration in which equilibrium is imposed is at time  $\vartheta = t + \Delta t/2$ . In this case, the relation between the kinematic variables becomes

$$\mathbf{u}_\vartheta = \frac{1}{2} (\mathbf{u}_t + \mathbf{u}_{t+\Delta t}) = \Delta \mathbf{u}_\vartheta; \quad (22)$$

$$\mathbf{v}_\vartheta = \frac{\mathbf{u}_{t+\Delta t} - \mathbf{u}_t}{\Delta t}; \quad (23)$$

$$\mathbf{a}_\vartheta = \frac{\mathbf{v}_{t+\Delta t} - \mathbf{v}_t}{\Delta t}. \quad (24)$$

In Eq. (22) it should be noted that initial displacements are null due to the introduction of a new mesh at the beginning of each time-step. The representation of the diverse configurations is given in Figure 1. In addition, the relationship between the deformation gradients appearing in the same figure is as follows

$$\mathbf{F} := \frac{\partial \mathbf{x}}{\partial \mathbf{X}} = \frac{\partial \mathbf{x}}{\partial \mathbf{x}_\vartheta} \frac{\partial \mathbf{x}_\vartheta}{\partial \tilde{\mathbf{X}}} \frac{\partial \tilde{\mathbf{X}}}{\partial \mathbf{X}} := \Delta \mathbf{F}_{\Delta t-\vartheta} \Delta \mathbf{F}_\vartheta \mathbf{F}_t. \quad (25)$$

It should be highlighted that  $\Delta(\bullet) := (\bullet)_{t+\Delta t} - (\bullet)_t$  usually indicates a difference between a quantity at the end of the step and its respective counterpart at the beginning, with the only exception being the deformation gradients  $\Delta \mathbf{F}_{\Delta t-\vartheta}$  and  $\Delta \mathbf{F}_\vartheta$ , which are defined by Eq. (25).

<sup>2</sup>It must be noted that the mid-point rule does not guarantee any conservation properties outside of the solution of the equilibrium equations, i.e., it does not apply to the mappings. This is the reason why mappings are assessed in Section 4 in terms of conservation properties.

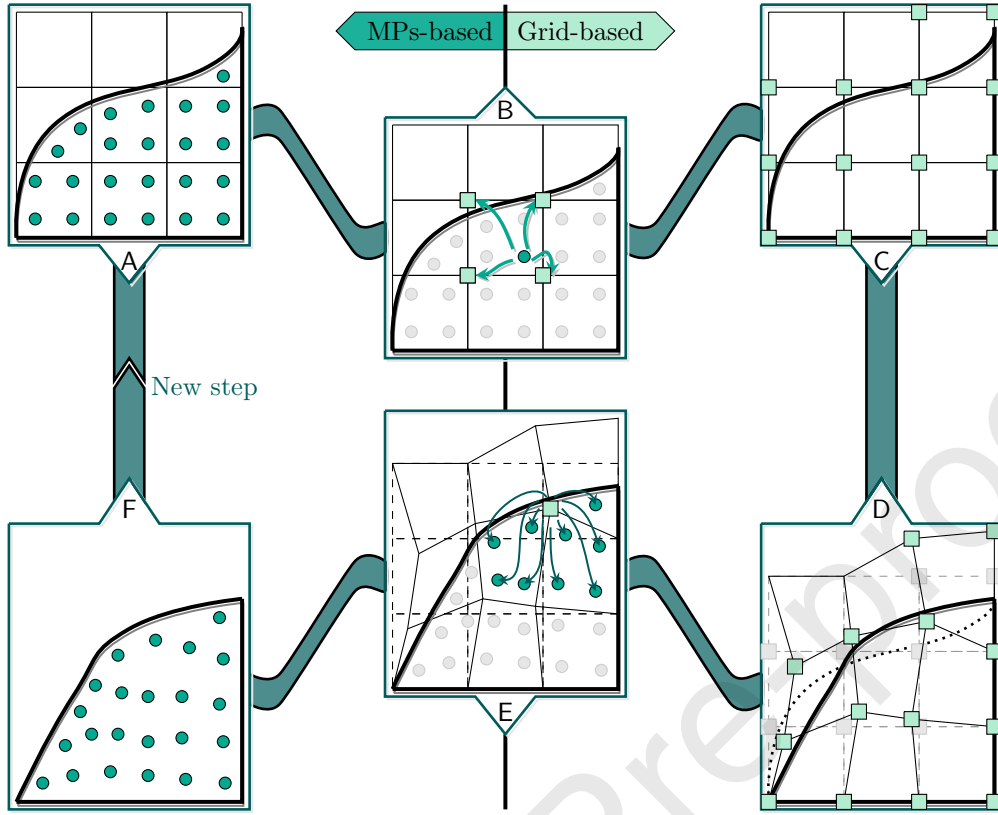


Fig. 2: An MPM main loop subdivided into procedural substeps for a single time-step. This loop is run until the simulation is complete at time  $T$ . On the left-hand side, there are the substeps involving the material points, while, on the right-hand side, the substeps using (mainly) the grid-based calculations. A loop comprises several steps: (A) current position of material points on the background grid, (B) point-to-grid information mapping, (C) equilibrium equations formulated at nodes on the grid, (D) solve equilibrium equations for nodal motion, (E) grid-to-point motion & deformation mapping and (F) deformed body in equilibrium with external actions and distorted grid disposal.

### 3. The Material Point Method algorithm structure

The main algorithmic steps for the MPM used here match previous descriptions (see, for instance, Coombs and Augarde [29]) and only significant features of steps pertinent to the new method are discussed here. Having established the continuum mechanics and discretisation approaches in the previous section, this section details the main algorithmic steps for a given time-step of the proposed implicit algorithm (as represented in Figure 2). The key steps A to E are described by Subsections 3.1 to 3.5. The final step, Step F, shows the deformed material point positions at the end of the loop, providing the starting point for the next loop through the algorithm.

#### 3.1. A: Discretisation - material points and grid initialisation

Regardless of the ontology, whether considering material points and the grid as two different and communicating discretisations or seeing them as a single one in which the two groups play different roles, the strength of the MPM lies in the presence of (simultaneous or discontinuous depending on the considered substeps) and the non-trivial communication between these two groups (material points and grid). Therefore, the initial conditions on the displacements and velocities required for the solution of Eqs. (20) and (21) can be prescribed independently on both the material

points and the grid. Due to the different mapping substeps, this information will be passed from one group to other (i.e., from the grid to the material points or vice versa).

### 3.2. B: Material points-to-grid mapping

A key issue for dynamic problems with the MPM is the need to maintain the same conservation properties (linear momentum, angular momentum and energies) of the material points representation as best as possible. The mapping procedures (substep B in Figure 2) from material points to grid proposed in the literature (see, among others, Love and Sulsky [19]) can be expressed as follows

$$\tilde{\mathbf{M}}_{IK} \mathbf{v}_K = \sum_{pt}^{N_{pt}} m^{pt} N_{Ii}(\mathbf{x}^{pt}) \mathbf{v}_i^{pt}. \quad (26)$$

The conservation properties of mapping (26) were investigated in 2006 by Love and Sulsky [19]. However, some of this is revisited in Subsection 4.1 below, to assess the conservation properties of the grid-to-material points mappings presented in Subsection 4.2.

### 3.3. C: Grid equilibrium equation assemblage

In this substep (C in Figure 2), Eqs. (20) and (21) are assembled at the grid nodes after having introduced the time discretisation explained in Subsection (2.3). As highlighted in [26; 30], the gradient of the shape functions must include the variation in deformation over the time-step to correctly enforce the equilibrium equations. Moreover, as can be seen from Eqs. (16) and (17), while the part of the external forces dealing with the body forces can be approximated via the integral over the chosen material points, the Neumann boundary conditions cannot be assembled in the same fashion within the MPM context; some suggested approaches are given in Bing *et al.* [31] and Remmerswaal [32]. In this work, when Neumann boundary conditions are considered (as in Example 7.1), concentrated loads are applied to selected material points, as explained in Charlton *et al.* [30].

### 3.4. D: Essential boundary conditions and solution procedure

The solution of Eq. (20) can take the same approach as the standard FE method where Dirichlet boundary conditions are directly applied on the grid (substep D in Figure 2). However, if the body boundaries (where the essential conditions are prescribed) do not match the grid, special techniques are necessary, such as proposed by Cortis *et al.* [33].

Iterative solutions to Eq. (20) are obtained via the Newton-Raphson algorithm, that is

$$\delta \mathbf{u}_{t+\Delta t}^{(k)} = - \left( \mathbf{J}^{(k-1)} \right)^{-1} \mathbf{r}^{(k-1)}, \quad (27)$$

where  $k$  indicates the current iteration,  $\delta \mathbf{u}_{t+\Delta t}^{(k)} := \mathbf{u}_{t+\Delta t}^{(k)} - \mathbf{u}_{t+\Delta t}^{(k-1)}$  are the incremental displacements, and  $\mathbf{J}^{(k-1)} := \frac{\partial \mathbf{r}}{\partial \mathbf{u}_{t+\Delta t}}$  is the Jacobian matrix. In the case of the mid-point rule, the full expression of this matrix is

$$\mathbf{J}^{(k-1)} = \frac{2}{\Delta t^2} \tilde{\mathbf{M}} + \mathbf{K}^{(k-1)},$$

with  $\mathbf{K}^{(k-1)} := \frac{\partial \mathbf{f}^{int}}{\partial \mathbf{u}_{t+\Delta t}}$  being the *global stiffness matrix*. Since the computation of the global stiffness matrix is strongly dependent on the stress-strain relationship (and the constitutive relationship is modified, as explained in Subsection 5.1), its calculation is fully detailed in Appendix A. It should be noted that the primary variable for Eq. (27) is arbitrary, while the update of the secondary unknowns should be made according to Eqs. (22) -(24).

Each time-step is considered to have converged once the ratio between the current error  $f^{Err}$  at the  $k$ -th iteration is less than a selected tolerance  $tol$  defined as

$$f^{Err} = \frac{(f^{Err})^{(k)}}{(f^{Err})^{(1)}} < tol, \quad \text{with} \quad (f^{Err})^{(k)} = (|\mathbf{r}^{(k)}|)_I (|\delta \mathbf{u}_{t+\Delta t}^{(k)}|)_I.$$

### 3.5. E: Grid-to-point mapping and update

Once the approximate solution to the equilibrium equation is found, it is necessary to pass the information from the grid to the material points (substep E in Figure 2). Moreover, if the characteristic function is not the Dirac delta function, an update of the function domain must be carried out (for a discussion and a comparison of the options, see Coombs *et al.* [26]).

For the material points-to-grid mapping in a dynamics problem, several options are available in the literature, which are PIC [8–10], FLIP [6; 7], XPIC [13], APIC [12; 34], and PolyPIC [14]. The current work focuses on the first two (PIC and FLIP) and highlights why the former is considered dissipative while the latter not (see Subsection 4.2). For the sake of completeness, the difference between the two is expressed by their update equations

$$\text{PIC:} \quad (\mathbf{v}_{t+\Delta t}^{pt})_i = \mathbf{N}_{il}(\mathbf{x}^{pt}) (\mathbf{v}_{t+\Delta t})_I; \quad (28)$$

$$\text{FLIP:} \quad (\mathbf{v}_{t+\Delta t}^{pt})_i = (\mathbf{v}_t^{pt})_i + \mathbf{N}_{il}(\mathbf{x}^{pt}) (\mathbf{v}_{t+\Delta t} - \mathbf{v}_t)_I. \quad (29)$$

The update of the material point current position is given by

$$(\mathbf{x}_{t+\Delta t}^{pt})_i = (\mathbf{x}_t^{pt})_i + \mathbf{N}_{il}(\mathbf{x}^{pt}) (\mathbf{u}_{t+\Delta t})_I = \mathbf{N}_{il}(\mathbf{x}^{pt}) (\mathbf{x}_{t+\Delta t})_I. \quad (30)$$

## 4. Properties of the mappings

The mapping procedures described by Eqs. (26), (28) and (29), which pass information back and forth, from the material points to the grid, are now assessed and their conservation of momenta (linear and angular) and of kinetic energy computed and reviewed. It should be emphasised that, theoretically, the goal of each mapping process is to conserve momenta and energy at the given time (i.e. the quantities of interest should be computed at the beginning or, alternatively, at the end of the step). However, as will be detailed in Subsection 4.1, the initial mapping inevitably loses energy at the beginning of each time-step. As a consequence, the objective of the mapping at the end of the time-step (i.e., grid-to-material points) changes in scope, having to eliminated (if possible) the error committed in the initial phase. For the grid-to-material points mapping process, the quantities of interest then become the time differences within the step. Therefore, it should be understood that, while the material points-to-grid mapping can be

defined as a unique process, the grid-to-material points cannot be decoupled from the mapping at the beginning of the step.

The Einstein summation notation has not been applied in Section 4 to make operations clearer, with the summation being explicit when necessary.

#### 4.1. The material points-to-grid mapping

The definitions of the momenta and kinetic energy computed on both the material points and the grid nodes are listed in Table 1. In particular, the former are denoted by the superscript  $(\bullet)^{pt}$ , while the latter by  $(\bullet)^h$ . Moreover, their differences, which were computed by Burgess *et al.* [11] for the consistent mass matrix and by Love and Sulsky [19] for the effective mass matrix, are reported in the same table.

Table 1: Definitions of material points' and grid linear momentum, angular momentum and kinetic energy. Their differences at the beginning of the step are computed using the mapping defined by Eq. (26).

| Quantities                    | Material Points'                                                                       | Grid                                                                                                                        | Difference                                         |
|-------------------------------|----------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------|
| Linear momentum $\mathbf{L}$  | $\mathbf{L}^{pt} := \sum_{pt}^{N_{pt}} m^{pt} \mathbf{v}^{pt};$                        | $\mathbf{L}^h := \sum_A^{N_{nodes}} \sum_B^{N_{nodes}} \tilde{\mathbf{M}}_{AB} (\mathbf{v}^h)_B;$                           | $\mathbf{L}_t^{pt} - \mathbf{L}_t^h = \mathbf{0};$ |
| Angular momentum $\mathbf{J}$ | $\mathbf{J}^{pt} := \sum_{pt}^{N_{pt}} \mathbf{x}^{pt} \times m^{pt} \mathbf{v}^{pt};$ | $\mathbf{J}^h := \sum_A^{N_{nodes}} (\mathbf{x}^h)_A \times \sum_B^{N_{nodes}} \tilde{\mathbf{M}}_{AB} (\mathbf{v}^h)_B;$   | $\mathbf{J}_t^{pt} - \mathbf{J}_t^h = \mathbf{0};$ |
| Kinetic energy $K$            | $K^{pt} := \frac{1}{2} \sum_{pt}^{N_{pt}} m^{pt} \ \mathbf{v}^{pt}\ ^2;^\dagger$       | $K^h := \frac{1}{2} \sum_A^{N_{nodes}} (\mathbf{v}^h)_A \cdot \sum_B^{N_{nodes}} \tilde{\mathbf{M}}_{AB} (\mathbf{v}^h)_B;$ | $K_t^{pt} - K_t^h \geq 0.$                         |

<sup>†</sup>  $\|(\bullet)\|$  is the Euclidean norm of  $(\bullet)$ .

To make the notation in Table 1 consistent with the definitions of mass matrices introduced by Eqs. (15), (18) and (19), it is useful to explain the relationship between them as follows.

$$\mathbf{M} = \int_{\Omega} \rho \underbrace{N_A \delta_{ki}}_{:=N_{Ii}} \delta_{ij} N_B d^h V = \int_{\Omega} \rho N_{Ii} N_{iK} d^h V, \quad (31)$$

with  $I = 1, \dots, (N_{Nodes} \times n^{dim}) = \mathbf{A} \times k = (1, \dots, N_{Nodes}) \times (1, \dots, n^{dim})$ .

Furthermore, from [19] the difference between material points' and grid kinetic energy for the mapping defined by Eq. (26), which, in Table 1 is generically expressed as greater or equal than zero, i.e.,

$$\begin{aligned} K_t^{pt} - K_t^h &= \frac{1}{2} \sum_{pt}^{N_{pt}} m^{pt} \|\mathbf{v}_t^{pt}\|^2 - \frac{1}{2} \sum_A^{N_{nodes}} (\mathbf{v}_t^h)_A \cdot \sum_B^{N_{nodes}} \tilde{\mathbf{M}}_{AB} (\mathbf{v}_t^h)_B \\ &= \frac{1}{2} \sum_{pt}^{N_{pt}} m^{pt} \|\mathbf{v}_t^{pt}\|^2 - \frac{1}{2} \sum_A^{N_{nodes}} (\mathbf{v}_t^h)_A \cdot \sum_B^{N_{nodes}} \mathbf{M}_{AB} (\mathbf{v}_t^h)_B \\ &\quad - \frac{\epsilon}{2} \sum_A^{N_{nodes}} (\mathbf{v}_t^h)_A \cdot \sum_B^{N_{nodes}} (\tilde{\mathbf{M}} - \mathbf{M})_{AB} (\mathbf{v}_t^h)_B \geq 0. \end{aligned} \quad (32)$$

Hence, the difference between the material points' and grid kinetic energy has a term (the third on the right-hand side) which is proportional to  $\epsilon$ . As such, it goes to zero when the consistent mass matrix is used in lieu of the effective mass matrix. However, the difference between the first term (material points' kinetic energy) and the second (proportional to

Table 2: Résumé of differences between time-increments computed on material points and grid using initial mapping (26) with FLIP, Eq. (29), or mapping (26) with PIC, Eq. (28).

| Differences                                    | Method           | Results                                                                                                                                                                                                                                                                                    |
|------------------------------------------------|------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| $\Delta \mathbf{L}^{pt} - \Delta \mathbf{L}^h$ | Eq. (26) + FLIP: | $= \mathbf{0};$                                                                                                                                                                                                                                                                            |
|                                                | Eq. (26) + PIC:  | $= \mathbf{0};$                                                                                                                                                                                                                                                                            |
| $\Delta \mathbf{J}^{pt} - \Delta \mathbf{J}^h$ | Eq. (26) + FLIP: | $= -\epsilon \sum_A^{N_{Nodes}} (\mathbf{x}_{t+\Delta t}^h)_A \times \sum_B^{N_{Nodes}} (\bar{\mathbf{M}} - \mathbf{M})_{AB} \Delta \mathbf{v}_B^h;$                                                                                                                                       |
|                                                | Eq. (26) + PIC:  | $= -\epsilon \sum_A^{N_{Nodes}} (\mathbf{x}_{t+\Delta t}^h)_A \times \sum_B^{N_{Nodes}} (\bar{\mathbf{M}} - \mathbf{M})_{AB} (\mathbf{v}_{t+\Delta t}^h)_B;$                                                                                                                               |
| $\Delta \mathbf{K}^{pt} - \Delta \mathbf{K}^h$ | Eq. (26) + FLIP: | $= -\frac{\epsilon}{2} \sum_A^{N_{Nodes}} \Delta \mathbf{v}_A^h \cdot \sum_B^{N_{Nodes}} (\bar{\mathbf{M}} - \mathbf{M})_{AB} \Delta \mathbf{v}_B^h;$                                                                                                                                      |
|                                                | Eq. (26) + PIC:  | $= -\frac{\epsilon}{2} \sum_A^{N_{Nodes}} \Delta \mathbf{v}_A^h \cdot \sum_B^{N_{Nodes}} (\bar{\mathbf{M}} - \mathbf{M})_{AB} (\mathbf{v}_{t+\Delta t}^h + \mathbf{v}_t^h)_B$<br>$-T_t^{pt} + \frac{1}{2} \sum_A^{N_{Nodes}} (\mathbf{v}_t^h)_A \cdot \mathbf{M}_{AB} (\mathbf{v}_t^h)_B.$ |

the consistent mass matrix) does not cancel out entirely. In particular, as shown by Burgess *et al.* [11], this difference is greater or equal to zero since material points are usually more numerous than grid nodes. As previously mentioned, this unavoidable error changes the goal of the grid-to-material points mapping at the end of the step.

#### 4.2. The grid-to-material points mapping

Differences of changes within the time-step between material points' and grid quantities for PIC and FLIP are reported in Table 2, where, in the case of FLIP, results were obtained by Love and Sulsky [19]. Hence, changes of momenta involving FLIP are only reported in Table 2, while the change in kinetic energy using FLIP is given for a detailed comparison with PIC. This comparative evaluation is necessary because the combination of the effective mass matrix with PIC is a new result, which agrees with the results of Burgess *et al.* [11] in the case of a lumped or a consistent matrix.

The difference between linear momentum values is (utilising Eqs. (28) and (18))

$$\begin{aligned}
 \Delta \mathbf{L}^{pt} - \Delta \mathbf{L}^h &= \mathbf{L}_{t+\Delta t}^{pt} - \mathbf{L}_{t+\Delta t}^h \\
 &= \sum_{pt}^{N_{pt}} m^{pt} \mathbf{v}_{t+\Delta t}^{pt} - \sum_A^{N_{nodes}} \sum_B^{N_{nodes}} \tilde{\mathbf{M}}_{AB} (\mathbf{v}_{t+\Delta t}^h)_B \\
 &= \sum_{pt}^{N_{pt}} m^{pt} \sum_B^{N_{Nodes}} N_B (\mathbf{v}_{t+\Delta t}^h)_A - (1 - \epsilon) \sum_{pt}^{N_{pt}} m^{pt} \underbrace{\sum_A^{N_{Nodes}} N_A}_{=1} \sum_B^{N_{Nodes}} N_B (\mathbf{v}_{t+\Delta t}^h)_B \\
 &\quad - \epsilon \sum_{pt}^{N_{pt}} m^{pt} \sum_B^{N_{Nodes}} N_B (\mathbf{v}_{t+\Delta t}^h)_B = \mathbf{0}.
 \end{aligned} \tag{33}$$

As it can be seen, PIC mapping conserves the linear momentum increment within the time-step. The difference between angular momenta is (with the contribution of Eqs. (30), (28), (15), and (18))

$$\Delta \mathbf{J}^{pt} - \Delta \mathbf{J}^h = \mathbf{J}_{t+\Delta t}^{pt} - \mathbf{J}_{t+\Delta t}^h$$

$$\begin{aligned}
&= \sum_{pt}^{N_{pt}} \mathbf{x}_{t+\Delta t}^{pt} \times m^{pt} \mathbf{v}_{t+\Delta t}^{pt} - \sum_A^{N_{nodes}} (\mathbf{x}_{t+\Delta t}^h)_A \times \sum_B^{N_{nodes}} \tilde{\mathbf{M}}_{AB} (\mathbf{v}_{t+\Delta t}^h)_B \\
&= \sum_{pt}^{N_{pt}} \sum_A^{N_{nodes}} N_A (\mathbf{x}_{t+\Delta t}^h)_A \times m^{pt} \sum_B^{N_{nodes}} N_B (\mathbf{v}_{t+\Delta t}^h)_B - \sum_A^{N_{nodes}} (\mathbf{x}_{t+\Delta t}^h)_A \times \sum_B^{N_{nodes}} \tilde{\mathbf{M}}_{AB} (\mathbf{v}_{t+\Delta t}^h)_B \\
&= \sum_A^{N_{nodes}} (\mathbf{x}_{t+\Delta t}^h)_A \times \sum_B^{N_{nodes}} (\mathbf{M} - \tilde{\mathbf{M}})_{AB} (\mathbf{v}_{t+\Delta t}^h)_B \\
&= -\epsilon \sum_A^{N_{nodes}} (\mathbf{x}_{t+\Delta t}^h)_A \times \sum_B^{N_{nodes}} (\tilde{\mathbf{M}} - \mathbf{M})_{AB} (\mathbf{v}_{t+\Delta t}^h)_B. \tag{34}
\end{aligned}$$

Eq. (34) shows that the difference is proportional to the velocity at the end of the step  $(\mathbf{v}_{t+\Delta t}^h)_I$ . This result is different from that obtained using FLIP, where the same quantity (see Table (2)) is proportional to the difference in velocities within the time-step  $(\Delta \mathbf{v}^h)_I$ . Therefore, the difference in angular momentum using PIC can be expected to be more significant, as the absolute velocity at the end of the step is likely to be greater in magnitude than the difference in velocity within the time-step. Nevertheless, in PIC and FLIP, errors are zero if the consistent mass matrix is employed. However, if the effective mass matrix is used, the difference in increment of angular momenta can decrease (dissipative behaviour) or increase.

Lastly, the difference between material points' and grid kinetic energy at the end of the step is computed, both for PIC (using contributions from Eqs. (28) and (15))

$$\begin{aligned}
K_{t+\Delta t}^{pt} - K_{t+\Delta t}^h &= \frac{1}{2} \sum_{pt}^{N_{pt}} m^{pt} \|\mathbf{v}_{t+\Delta t}^{pt}\|^2 - \frac{1}{2} \sum_A^{N_{nodes}} (\mathbf{v}_{t+\Delta t}^h)_A \cdot \sum_B^{N_{nodes}} \tilde{\mathbf{M}}_{AB} (\mathbf{v}_{t+\Delta t}^h)_B \\
&= \frac{1}{2} \sum_{pt}^{N_{pt}} m^{pt} \left( \sum_A^{N_{nodes}} N_A (\mathbf{v}_{t+\Delta t}^h)_A \right) \cdot \left( \sum_B^{N_{nodes}} N_B (\mathbf{v}_{t+\Delta t}^h)_B \right) - \frac{1}{2} \sum_A^{N_{nodes}} (\mathbf{v}_{t+\Delta t}^h)_A \cdot \sum_B^{N_{nodes}} \tilde{\mathbf{M}}_{AB} (\mathbf{v}_{t+\Delta t}^h)_B \\
&= \frac{1}{2} \sum_A^{N_{nodes}} (\mathbf{v}_{t+\Delta t}^h)_A \cdot \sum_B^{N_{nodes}} \underbrace{(\mathbf{M} - \tilde{\mathbf{M}})_{AB}}_{=-\epsilon(\tilde{\mathbf{M}} - \mathbf{M})_{AB}} (\mathbf{v}_{t+\Delta t}^h)_B \leq 0, \tag{35}
\end{aligned}$$

and FLIP (by using Eqs. (29), (15), and (26))

$$\begin{aligned}
K_{t+\Delta t}^{pt} - K_{t+\Delta t}^h &= \frac{1}{2} \sum_{pt}^{N_{pt}} m^{pt} \|\mathbf{v}_{t+\Delta t}^{pt}\|^2 - K_{t+\Delta t}^h \\
&= \frac{1}{2} \sum_{pt}^{N_{pt}} m^{pt} \left( \mathbf{v}_t^{pt} + \sum_A^{N_{nodes}} N_A \Delta \mathbf{v}_A^h \right) \cdot \left( \mathbf{v}_t^{pt} + \sum_B^{N_{nodes}} N_B \Delta \mathbf{v}_B^h \right) - K_{t+\Delta t}^h \\
&= \frac{1}{2} \sum_{pt}^{N_{pt}} m^{pt} \|\mathbf{v}_t^{pt}\|^2 + \frac{1}{2} \sum_{pt}^{N_{pt}} m^{pt} \left( \sum_A^{N_{nodes}} N_A \Delta \mathbf{v}_A^h \right) \cdot \left( \sum_B^{N_{nodes}} N_B \Delta \mathbf{v}_B^h \right) + \sum_{pt}^{N_{pt}} m^{pt} \mathbf{v}_t^{pt} \cdot \left( \sum_A^{N_{nodes}} N_A \Delta \mathbf{v}_A^h \right) - K_{t+\Delta t}^h \\
&= K_t^{pt} + \frac{1}{2} \sum_{A,B}^{N_{nodes}} \Delta \mathbf{v}_A^h \cdot \mathbf{M}_{AB} \Delta \mathbf{v}_B^h + \sum_{A,B}^{N_{nodes}} \Delta \mathbf{v}_A^h \cdot \tilde{\mathbf{M}}_{AB} (\mathbf{v}_t^h)_B - K_{t+\Delta t}^h \\
&= K_t^{pt} + \frac{1}{2} \sum_{A,B}^{N_{nodes}} \left( (\mathbf{v}_{t+\Delta t}^h)_A \cdot \mathbf{M}_{AB} (\mathbf{v}_{t+\Delta t}^h)_B + (\mathbf{v}_t^h)_A \cdot \mathbf{M}_{AB} (\mathbf{v}_t^h)_B - 2 (\mathbf{v}_{t+\Delta t}^h)_A \cdot \mathbf{M}_{AB} (\mathbf{v}_t^h)_B + 2 (\mathbf{v}_{t+\Delta t}^h)_A \cdot \tilde{\mathbf{M}}_{AB} (\mathbf{v}_t^h)_B \right)
\end{aligned}$$

$$\begin{aligned}
& -2 \left( \mathbf{v}_t^h \right)_A \cdot \tilde{\mathbf{M}}_{AB} \left( \mathbf{v}_t^h \right)_B - \left( \mathbf{v}_{t+\Delta t}^h \right)_A \cdot \tilde{\mathbf{M}}_{AB} \left( \mathbf{v}_{t+\Delta t}^h \right)_B \\
& = K_t^{pt} - K_t^h + \frac{1}{2} \sum_{A,B}^{N_{Nodes}} \Delta \mathbf{v}_A^h \cdot \underbrace{(\mathbf{M} - \tilde{\mathbf{M}})_{AB}}_{=-\epsilon(\tilde{\mathbf{M}} - \mathbf{M})_{AB}} \Delta \mathbf{v}_B^h.
\end{aligned} \tag{36}$$

It should be noted that the inequality in Eq. (35) was proven previously in Love and Sulsky [19] via positive semi-definiteness of the symmetric quantity  $\tilde{\mathbf{M}} - \mathbf{M}$ . Suppose we consider Eqs. (35) and (36), we should see that, in the case of a consistent matrix, PIC would appear to be energy-conservative, while FLIP would repeat the error made at the beginning of the time-step. However, by virtue of the error quantified by Eq. (32), Eqs. (35) and (36) are not of interest but the combination of these latter with Eq. (32) is. In the case of PIC, this calculations is

$$\begin{aligned}
\Delta K^{pt} - \Delta K^h &= \underbrace{K_{t+\Delta t}^{pt} - K_{t+\Delta t}^h}_{\leq 0} - \underbrace{(K_t^{pt} - K_t^h)}_{\leq 0} \\
&= -\frac{\epsilon}{2} \sum_A^{N_{Nodes}} \left( \mathbf{v}_{t+\Delta t}^h \right)_A \cdot \sum_B^{N_{Nodes}} (\tilde{\mathbf{M}} - \mathbf{M})_{AB} \left( \mathbf{v}_{t+\Delta t}^h \right)_B - \frac{1}{2} \sum_{pt}^{N_{pt}} m^{pt} \left\| \mathbf{v}_t^{pt} \right\|^2 + \frac{1}{2} \sum_A^{N_{Nodes}} \left( \mathbf{v}_t^h \right)_A \cdot \sum_B^{N_{Nodes}} \mathbf{M}_{AB} \left( \mathbf{v}_t^h \right)_B \\
&\quad + \frac{\epsilon}{2} \sum_A^{N_{Nodes}} \left( \mathbf{v}_t^h \right)_A \cdot \sum_B^{N_{Nodes}} (\tilde{\mathbf{M}} - \mathbf{M})_{AB} \left( \mathbf{v}_t^h \right)_B \\
&= -\frac{\epsilon}{2} \sum_A^{N_{Nodes}} \Delta \mathbf{v}_A^h \cdot \sum_B^{N_{Nodes}} (\tilde{\mathbf{M}} - \mathbf{M})_{AB} \left( \mathbf{v}_{t+\Delta t}^h + \mathbf{v}_t^h \right)_B - T_t^{pt} + \frac{1}{2} \sum_A^{N_{Nodes}} \left( \mathbf{v}_t^h \right)_A \cdot \mathbf{M}_{AB} \left( \mathbf{v}_t^h \right)_B \leq 0.
\end{aligned} \tag{37}$$

The same process (first described by Love and Sulsky [18]) can be applied to the FLIP method using Eqs. (36) and (32), i.e.,

$$\begin{aligned}
\Delta K^{pt} - \Delta K^h &= K_{t+\Delta t}^{pt} - K_{t+\Delta t}^h - (K_t^{pt} - K_t^h) \\
&= -\frac{\epsilon}{2} \sum_A^{N_{Nodes}} (\Delta \mathbf{v}_A^h) \cdot \sum_B^{N_{Nodes}} (\tilde{\mathbf{M}} - \mathbf{M})_{AB} \Delta \mathbf{v}_B^h \leq 0.
\end{aligned} \tag{38}$$

As Eqs. (37) and (38) show, while FLIP can cancel the kinetic energy difference from the initial mapping procedure, PIC cannot. Hence, PIC is not dissipative per se, but the combination of the initial mapping defined by Eq. (26) with PIC (28) leads to dissipation at the end of the step, even when the consistent mass matrix is used. On the other hand, the combination of Eq. (26) with FLIP (29) does not lead to kinetic energy dissipation, as the initial difference is mathematically cancelled in the consistent mass matrix case.

In addition, since linear and angular momentum and kinetic energy do not depend on acceleration but only on velocity (linear momentum and kinetic energy) or position (angular momentum), there is no need to map the acceleration at the end of the time-step to ensure conservation. However, these mappings (back and forth) are sometimes performed (as in, for instance, Iaconeta *et al.* [35]) for the post-processing phase and to have the initial acceleration at the beginning of the time-step  $\mathbf{a}_i$  non-zero.

## 5. Properties of the Updated Lagrangian formulation

A key part of an implicit MPM formulation is calculation of the internal force vector and for the new method this is needed in the updated Lagrangian frame. As can be seen from Eq. (13), the most compact and natural writing of this internal force vector uses the Cauchy stress tensor  $\sigma$  or, similarly, the Kirchhoff stress tensor  $\tau^3$ , as shown in Eq. (3). Therefore, the second Piola-Kirchhoff stress tensor's modified definition  $S^{mp}$  (firstly proposed by Simo and Tarnow [20]) is pushed forward to the current configuration to obtain its analogue in Kirchhoff form  $\tau^{mp}$ . Once this operation is performed, all conservation properties (momenta and strain energy conservation) related to  $S^{mp}$  are transferred to  $\tau^{mp}$ . The reader interested in the proofs of the conservation properties is referred to Simo and Tarnow [20] or Love and Sulsky [18; 19].

To move the reference configuration, the internal force vector, expressed in a total Lagrangian formulation, is given from [20] as

$$\mathbf{F}_{\theta}^{int} = \int_{\Omega_0} (\nabla_X \mathbf{N})^T \mathbf{F}_{\theta} S^{mp} dV_0, \quad (39)$$

with  $S^{mp}$  being the energy-consistent second Piola-Kirchhoff stress tensor. The transition from a total Lagrangian formulation to an updated Lagrangian formulation leads to a change in the integration volume, i.e.,

$$\mathbf{f}_{\theta}^{int} = \int_{\Omega_{t+\Delta t}} (\nabla_X \mathbf{N})^T \mathbf{F}_{\theta} S^{mp} (J_{t+\Delta t})^{-1} dV_{t+\Delta t}. \quad (40)$$

Moreover, it is useful to express the following quantities as

$$\nabla_X \mathbf{N} = \frac{\partial \mathbf{N}}{\partial \mathbf{X}} = \frac{\partial \mathbf{N}}{\partial \mathbf{x}} \frac{\partial \mathbf{x}}{\partial \mathbf{X}} = \nabla_x \mathbf{N} \mathbf{F}; \quad (41)$$

$$\mathbf{F}_{t+\theta} = \frac{\partial \mathbf{x}_{t+\theta}}{\partial \mathbf{X}} = \frac{\partial \mathbf{x}_{t+\theta}}{\partial \tilde{\mathbf{X}}} \frac{\partial \tilde{\mathbf{X}}}{\partial \mathbf{X}} = \Delta \mathbf{F}_{\theta} \mathbf{F}_t. \quad (42)$$

By using the above equations and the definition of the Kirchhoff stress in the current configuration, which is

$$\mathbf{S}^{mp} = (\mathbf{F})^{-1} \tau^{mp} (\mathbf{F})^{-T}, \quad (43)$$

the internal force vector defined by Eq. 40 becomes

$$\mathbf{f}_{\theta}^{int} = \int_{\Omega_{t+\Delta t}} (\nabla_x \mathbf{N})^T \underbrace{\Delta \mathbf{F}_{\theta} \mathbf{F}_t (\mathbf{F})^{-1}}_{=(\Delta \mathbf{F}_{\Delta t-\theta})^{-1}} \tau^{mp} \underbrace{(J_{t+\Delta t})^{-1} dV_{t+\Delta t}}_{=dV_0}. \quad (44)$$

It should be noted that Eq. (44) is not a unique choice, since the Kirchhoff stress could be mapped to the intermediate configuration. This discrepancy between the configuration where the equilibrium is imposed (i.e., intermediate) and the one where the algorithmic Kirchhoff stress lives (i.e., the current configuration) leads the stress tensor

<sup>3</sup>The authors recognise the importance of the study proposed by Bennet *et al.* [36] in which it is shown that an Eshelby-like stress tensor is the only one that satisfies both the second law of thermodynamics and the assumption of an intermediate stress-free configuration. However, in light of the same argument advanced by Choo and Sun [37] and in line with the tradition of the Kirchhoff tensor as a measure for plasticity at finite deformation (see, among others, de Souza Neto *et al.* [38]), the present work adopts the Kirchhoff tensor as the stress measure for the proposed updated Lagrangian framework. The Kirchhoff measure does not violate the second law of thermodynamics and therefore remains an excellent candidate for an energy-conserving MPM formulation.

( $\Delta \mathbf{F}_{\Delta t-\theta}$ )<sup>-1</sup>  $\boldsymbol{\tau}^{mp}$  to be asymmetric (see, for a detailed discussion, Marsden and Hughes [39]). Despite this additional complication, the decision to push the Kirchhoff stress to the current configuration seems more streamlined, especially as the linearisation of  $\boldsymbol{\tau}^{mp}$  is independent from the considered intermediate configuration, which, if time integration schemes different from the mid-point rule are considered, can vary between the previously converged and the current one.

### 5.1. Stress-strain modified relationship

As mentioned above, the stress-strain relationship used above does not dissipate energy within the framework of finite deformation theory. In this work, power conjugates are used to establish how this modification changes when the stress tensor is the Kirchhoff tensor, i.e.,  $\frac{1}{2} \mathbf{S} : \dot{\mathbf{C}} = \boldsymbol{\tau} : \mathbf{d}$ , with  $\mathbf{C} := \mathbf{F}^T \mathbf{F}$  being the right Cauchy-Green tensor, and  $\mathbf{d} := (\dot{\mathbf{F}} \mathbf{F}^{-1} + (\dot{\mathbf{F}} \mathbf{F}^{-1})^T) / 2$  the rate of deformation tensor. As incremental relationships are substituted by time-discretised ones, the time-difference of the right Cauchy-Green tensor  $\Delta \mathbf{C}$  is related to the averaged (over the time-step) rate of the deformation tensor, denoted as  $\bar{\mathbf{d}}$ . Therefore, The time-discretised power conjugates become

$$\frac{1}{2} \mathbf{S}^{mp} : \Delta \mathbf{C} = \boldsymbol{\tau}^{mp} : \bar{\mathbf{d}}. \quad (45)$$

Hence, by using Eq. (43), the definition of  $\bar{\mathbf{d}}$  is

$$\bar{\mathbf{d}} := \frac{1}{2} \mathbf{F}^{-T} \Delta \mathbf{C} \mathbf{F}^{-1}. \quad (46)$$

The modified stress-strain relationship for a Hencky material using  $\mathbf{S}^{mp4}$  is here recalled

$$\mathbf{S}^{mp} = \frac{1}{2} (\mathbf{S}_t + \mathbf{S}_{t+\Delta t}) + \underbrace{\frac{\Delta \mathbf{C}}{\|\Delta \mathbf{C}\|^2} \left( 2 (\Delta \psi + \Delta \mathcal{D}^{int}) - \frac{1}{2} (\mathbf{S}_t + \mathbf{S}_{t+\Delta t}) : \Delta \mathbf{C} \right)}_{:= \Delta \mathcal{H}^{int}}, \quad (47)$$

where  $\Delta \psi = \psi_{t+\Delta t} - \psi_t$  is the difference in the free energy function  $\psi$ . The difference in internal dissipation  $\Delta \mathcal{D}^{int}$  is, if associative flow rules are considered, given by

$$\Delta \mathcal{D}^{int} = \Delta \gamma \left( \boldsymbol{\tau}_{t+\Delta t} : \frac{\partial \Phi}{\partial \boldsymbol{\tau}_{t+\Delta t}} + q_{t+\Delta t} \frac{\partial \Phi}{\partial q_{t+\Delta t}} \right),$$

with  $q := -\frac{\partial \psi}{\partial \xi}$  being a scalar hardening variable and  $\xi$  its conjugate responsible for isotropic hardening. By pre-multiplying by  $\mathbf{F}$  and post-multiplying by  $\mathbf{F}^T$  the Eq. 47, the stress strain-relationship can be written using  $\boldsymbol{\tau}^{mp}$ , i.e.,

$$\begin{aligned} \boldsymbol{\tau}^{mp} &= \mathbf{F} \mathbf{S}^{mp} \mathbf{F}^T = \frac{1}{2} \mathbf{F} (\mathbf{S}_t + \mathbf{S}_{t+\Delta t}) \mathbf{F}^T + \mathbf{F} \Delta \mathbf{C} \mathbf{F}^T \left( \frac{\Delta \mathcal{H}^{int}}{\|\Delta \mathbf{C}\|^2} \right) = \\ &= \frac{1}{2} \underbrace{\mathbf{F} \mathbf{S}_t \mathbf{F}^T}_{= \Delta \mathbf{F} \boldsymbol{\tau}_t \Delta \mathbf{F}^T} + \frac{1}{2} \boldsymbol{\tau}_{t+\Delta t} + \mathbf{F} \Delta \mathbf{C} \mathbf{F}^T \left( \frac{\Delta \mathcal{H}^{int}}{\|\Delta \mathbf{C}\|^2} \right) = \bar{\boldsymbol{\tau}} + \mathbf{F} \Delta \mathbf{C} \mathbf{F}^T \left( \frac{\Delta \mathcal{H}^{int}}{\|\Delta \mathbf{C}\|^2} \right), \end{aligned} \quad (48)$$

<sup>4</sup>The definition (47) comes originally from Gonzalez [21], but the additive term  $\Delta \mathcal{D}^{int}$  to include plastic dissipation was added by Meng and Laursen [24]. Moreover, the definition of an algorithmic stress tensor which satisfies the conservation of energy is not unique, as underlined by Armero and Romero [22]: there exist several formulations of discrete derivatives which conserve *directionality* and *consistency* (for a detailed discussion, see Love and Sulsky [18]).

where the trapezoidal stress  $\bar{\tau}$  has been defined as

$$\bar{\tau} := \frac{1}{2} \mathbf{F} (\mathbf{S}_t + \mathbf{S}_{t+\Delta t}) \mathbf{F}^T = \frac{1}{2} (\Delta \mathbf{F} \boldsymbol{\tau}_t \Delta \mathbf{F}^T + \boldsymbol{\tau}_{t+\Delta t}) = \frac{1}{2} (\boldsymbol{\tau}_t^{PF} + \boldsymbol{\tau}_{t+\Delta t}). \quad (49)$$

In the above equation, the quantity  $\boldsymbol{\tau}_t^{PF} = \Delta \mathbf{F} \boldsymbol{\tau}_t \Delta \mathbf{F}^T$  corresponds to the Kirchhoff stress evaluated at the previous step  $\boldsymbol{\tau}_t$ , pushed forward to the current configuration. This is in compliance with the current Kirchhoff stress  $\boldsymbol{\tau}_{t+\Delta t}$ , which lives in the current configuration.

It is useful to consider what physical quantity corresponds to the product  $\mathbf{F} \Delta \mathbf{C} \mathbf{F}^T$ . To proceed, let us introduce the left Cauchy-Green tensor  $\mathbf{b} := \mathbf{F} \mathbf{F}^T$ , so it follows that

$$\begin{aligned} F_{ih} (\Delta \mathbf{C})_{hk} F_{jk} &= F_{ih} (C_{hk} - (C_t)_{hk}) F_{jk} = F_{ih} F_{ah} F_{ak} F_{jk} - \Delta F_{i\beta} (F_t)_{\beta h} (F_t)_{ah} (F_t)_{ak} \Delta F_{j\gamma} (F_t)_{\gamma k} \\ &= b_{ia} b_{aj} - \Delta F_{i\beta} (b_t)_{\beta\alpha} (b_t)_{\alpha\gamma} \Delta F_{j\gamma} := \Delta^{PF} b_{ij}, \end{aligned} \quad (50)$$

where, when the reference configuration is omitted, the quantities are referred to the current time  $t + \Delta t$ . Owing to the above equation, the quantity  $\mathbf{F} \Delta \mathbf{C} \mathbf{F}^T$  can be seen as a difference between the squared current left Cauchy-Green strain tensor  $\mathbf{b}$  and the same quantity evaluated at the previous step  $\mathbf{b}_t$  which has been pushed forward as a contravariant tensor. Therefore, Eq. (48) can be rewritten as

$$\boldsymbol{\tau}^{mp} = \bar{\tau} + \Delta^{PF} \mathbf{b} \left( \frac{\Delta \mathcal{H}^{int}}{\|\Delta \mathbf{C}\|^2} \right). \quad (51)$$

It can be shown that the following energy inequality holds for the finite work within the step defined by algorithmic stress tensor (51) and its conjugate kinematic variable (46), which is

$$\frac{1}{2} \mathbf{S}^{mp} : \Delta \mathbf{C} = \boldsymbol{\tau}^{mp} : \bar{\mathbf{d}} = \Delta \psi + \Delta \mathcal{D}^{int} \geq \Delta \mathcal{D}^{int}. \quad (52)$$

Owing to Eqs. (48) and (46), it follows that

$$\begin{aligned} \boldsymbol{\tau}^{mp} : \bar{\mathbf{d}} &= \left( \frac{1}{2} (\boldsymbol{\tau}_t^{PF} + \boldsymbol{\tau}_{t+\Delta t}) + \mathbf{F} \Delta \mathbf{C} \mathbf{F}^T \left( \frac{\Delta \mathcal{H}^{int}}{\|\Delta \mathbf{C}\|^2} \right) \right) : \frac{1}{2} (\mathbf{F}^{-T} \Delta \mathbf{C} \mathbf{F}^{-1}) \\ &= \frac{1}{4} (\boldsymbol{\tau}_t^{PF} + \boldsymbol{\tau}_{t+\Delta t}) : (\mathbf{F}^{-T} \Delta \mathbf{C} \mathbf{F}^{-1}) + \frac{1}{2} \frac{\Delta \mathcal{H}^{int}}{\|\Delta \mathbf{C}\|^2} (\mathbf{F} \Delta \mathbf{C} \mathbf{F}^T : \mathbf{F}^{-T} \Delta \mathbf{C} \mathbf{F}^{-1}). \end{aligned} \quad (53)$$

The following simplifications can be made

$$\mathbf{F} \Delta \mathbf{C} \mathbf{F}^T : \mathbf{F}^{-T} \Delta \mathbf{C} \mathbf{F}^{-1} = \Delta \mathbf{C} : \Delta \mathbf{C}; \quad (54)$$

$$\frac{1}{2} (\mathbf{S}_t + \mathbf{S}_{t+\Delta t}) : \Delta \mathbf{C} = (\mathbf{S}_t + \mathbf{S}_{t+\Delta t}) : \mathbf{F}^T \bar{\mathbf{d}} \mathbf{F} = (\Delta \mathbf{F} \boldsymbol{\tau}_t \Delta \mathbf{F}^T + \boldsymbol{\tau}_{t+\Delta t}) : \bar{\mathbf{d}} = 2 \bar{\tau} : \bar{\mathbf{d}}. \quad (55)$$

Therefore, the quantity  $\Delta \mathcal{H}^{int}$  in the Eq. (51) can be rewritten as

$$\Delta \mathcal{H}^{int} = 2 (\Delta \psi + \Delta \mathcal{D}^{int}) - \frac{1}{2} (\mathbf{S}_t + \mathbf{S}_{t+\Delta t}) : \Delta \mathbf{C} = 2 (\Delta \psi + \Delta \mathcal{D}^{int}) - 2 \bar{\tau} : \bar{\mathbf{d}}.$$

By the use of Eqs. (54) and (56), inequality (52) can be verified

$$\begin{aligned}
 \tau^{mp} : \bar{\mathbf{d}} &= \frac{1}{2} (\tau_t^{PF} + \tau_{t+\Delta t}) : \bar{\mathbf{d}} + \frac{1}{2 \|\Delta \mathbf{C}\|^2} (2 (\Delta \psi + \Delta \mathcal{D}^{int}) - 2 \bar{\tau} : \bar{\mathbf{d}}) \Delta \mathbf{C} : \Delta \mathbf{C} \\
 &= \bar{\tau} : \bar{\mathbf{d}} + (\Delta \psi + \Delta \mathcal{D}^{int}) - \bar{\tau} : \bar{\mathbf{d}} \\
 &= \Delta \psi + \Delta \mathcal{D}^{int} \geq \Delta \psi.
 \end{aligned} \tag{56}$$

## 6. Adaptive time-step length based on the Courant-Friedrich-Lewy condition

For computational efficiency and stability, the choice of time-step size is important regardless of temporal discretisation. The maximum time-step size in explicit solution techniques is limited by the well-known CFL condition

$$\Delta t^{CFL} = \min_i (h_i^h) \sqrt{\frac{\rho}{M}}, \tag{57}$$

where  $h_i^h$  is the mesh size in the  $i$ -th direction ( $\in \mathbb{R}^{n^{dim}}$ ), and  $\rho$  and  $M$  are the density and the P-wave modulus of the material being analysed. The above equation holds for any body under the assumption of small strains or for underformed Hencky materials within the finite strain theory. While the adaptation of this formula to deformed bodies within finite strain theory has been carried out by Sun *et al.* [40], this work underlines that, within the MPM, the CFL condition is not a steady quantity in the simulation, as some grid elements can be entirely filled with material points, while others only partially. Hence, when mapping information (masses and mechanical properties) from material points to grid nodes, the grid-averaged values of these quantities coming from partially filled elements are smaller than those coming from entirely filled elements. This variability in mass and stiffness affects the CFL limitation on the time-step size *during* the analysis. For implicit temporal discretisations, the CFL condition is not required to guarantee method stability however it can be used to provide an adaptive time-step size for efficiency. Understanding how this condition varies during a simulation is therefore, if not necessary is at least practical for adapting the time-step length.

To the authors' knowledge, these considerations are new within the MPM framework, but they are well-recognised, for instance, in the cut finite element method (see Sticko *et al.* [41]) where a generalised eigenvalue problem of the discrete linear momentum conservation (Eq. (21)) is solved to compute the CFL condition. In this work we adopt a convenient computational simplification, which relies on the mapping at the beginning of the step. The CFL constraint in Eq. (57) can be mapped at the beginning of the step from the material points (where information such as density and elastic moduli lie) to the grid nodes as follows

$$m_A^h = \sum_{pt}^{N_{pt}} N_A m^{pt}; \tag{58}$$

$$V_A^h = \sum_{pt}^{N_{pt}} N_A V^{pt}; \tag{59}$$

$$M_A^h = \sum_{pt}^{N_{pt}} N_A M^{pt}, \tag{60}$$

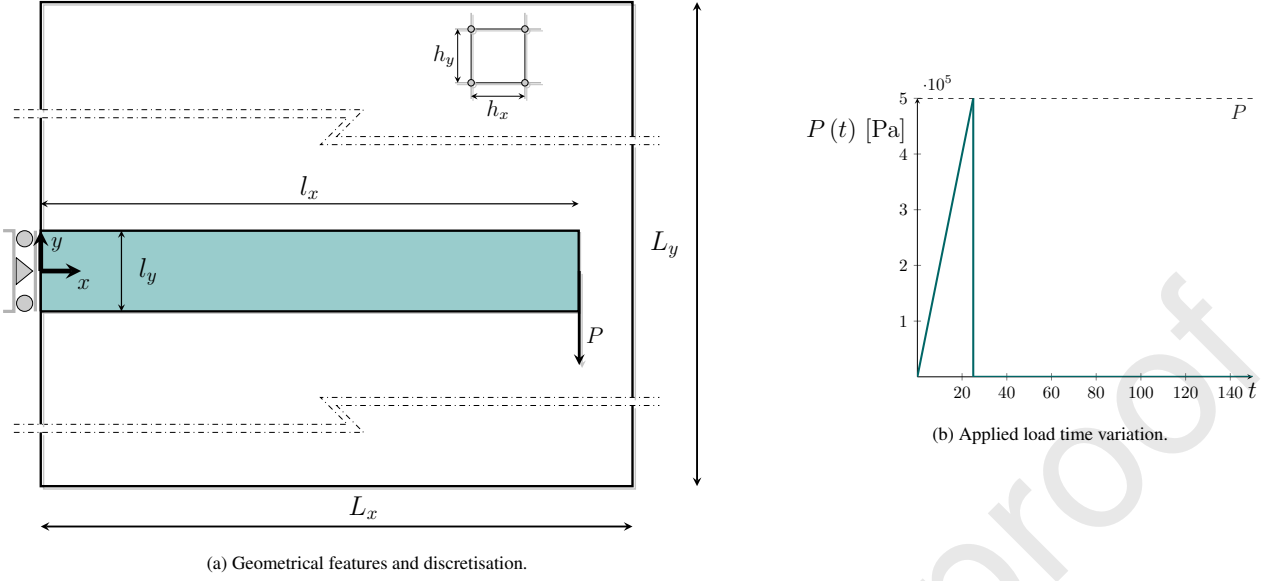


Fig. 3: The cantilever beam problem.

In this fashion, a grid-averaged value of these quantities is computed. Hence, the computation of the approximated time-step length based on the CFL condition becomes

$$\Delta t^{CFL} \approx \min_i (h_i^h) \min_A \left( \sqrt{\frac{m^h}{V^h M^h}} \right)_A, \quad \text{with } A = 1, \dots, N_{nodes}. \quad (61)$$

Eq. (61) has to be intended as a rule of thumb more than as a strict rule, making it valuable for adapting the time-step in implicit schemes.

## 7. Numerical examples

The method outlined in the previous sections is applied here to three examples of low-frequency dynamic problems. In compliance with the assumptions introduced in Section 2, the following numerical analyses consider a Hencky material. Since the aim of this work is to consider under which conditions energy and momenta are conserved, in accordance with Section 4, the consistent mass matrix (15) together with a FLIP mapping (29) are always used for the following numerical simulations. The time-step length was adapted manually for the different examples, remaining several times larger than the CFL condition value, without compromising optimal Newton-Raphson convergence. Moreover, the error tolerances ( $tol$ ) have been set to a strict value of  $10^{-11}$  to demonstrate the strong convergence behaviour of the proposed method.

### 7.1. 2D elastic cantilever beam

The first example is a bi-dimensional elastic beam represented in Figure 3a. In particular, two analyses with different elastic parameters were run, the former, i.e., (A), with a compressible material, and the latter, i.e., (B) with a nearly-incompressible material. The analyses were run using GIMPM instead of the original MPM formulation.

Table 3: Summary of the parameters considered in the analyses of the 2D elastic cantilever beam.

| Parameter Settings         |                 | Analysis (A)                        | Analysis (B)       |
|----------------------------|-----------------|-------------------------------------|--------------------|
| Material Parameters        | $E$             | $10^9$ Pa                           | $3 \cdot 10^8$ Pa  |
|                            | $\nu$           | 0.2                                 | 0.49               |
|                            | $\rho$          | $7750 \cdot 10^3$ kg/m <sup>3</sup> |                    |
| Geometry, Load and Timings | $l_x, l_y$      | 10, 1 m                             |                    |
|                            | $P$             | 500 kN                              |                    |
|                            | $t_0, t_1, T$   | 0, 25, 150 s                        |                    |
| Analysis Parameters        | $L_x, L_y$      | 11, 20 m                            |                    |
|                            | $h_x, h_y$      | 0.5 m                               |                    |
|                            | $^{\dagger}mmp$ | 12                                  |                    |
|                            | $\Delta t$      | $\approx 0.6264$ s                  | $\approx 0.2194$ s |

<sup>†</sup>  $mmp$  is the number of material points per direction per element.

As illustrated in Figure 3b, the load, applied at the end of the free edge, is monotonically increased from 0 to its highest value  $P$  and then suddenly removed. The peak value of the load is reached at the time  $t_1 = 25$  s, while the whole simulation carries on until time  $T = 150$  s. The effects of gravity were neglected. The external load vector is represented by the point load, which is split between the two end material points in the proximity of the  $x$ -axis. The material parameters, beam geometry and discretisation for the current two variants, i.e., analyses (A) and (B), are summarised in Table 3. In particular, the incremental time lengths  $\Delta t$  shown in Table 1 correspond to 15 times the CFL time-step approximation defined at the beginning of the simulation by Eq. (57). Moreover, it can be noticed how the number of material points per element is particularly high. The reason of such an unusual number lies in one of the most common issues for the MPM, namely the integration error (see, for instance, Yamaguchi *et al.* [42] or Gan *et al.* [43]). This integration error is particularly evident when a grid node is active only due a single and misplaced (from an integration position perspective) material point. In this case, the badly-integrated quantity will present very small entry relative to that nodes. In turn, this small entries can give numerical difficulties when it is necessary to invert the badly-integrated quantity (as in the case of the mass matrix or the stiffness matrix). As predictable, this situation is less likely to occur if the mesh is pretty coarse and the number of material points per element is high, as less likely is the chance of an unique material point mapping to a given node. The chance of experiencing this issue can increase with the order of the shape functions, as bigger is their relative stencil.

The periodic behaviour of the structure's energies is reported in Figure 4a for analysis (A), where total, material points' kinetic, and strain energy are considered. The time-steps denoted by letters in the same figure correspond to sensitive configurations: the last time-step where the load is applied before its removal ( $A \approx 24.43$  s, 39<sup>th</sup> time-step), the maximum value of the strain energy ( $B \approx 29.44$  s, 47<sup>th</sup> time-step, and  $D \approx 55.12$  s, 88<sup>th</sup> time-step), and the maximum value of the kinetic energy ( $C \approx 42.59$  s, 68<sup>th</sup> time-step). As shown in Figures 4b and 4c, after the load is removed (just after time-step A), the beam continues to move downwards until the inertia is wholly converted into strain energy (Figures 4d and 4e, time-step B). As expected, Figure 4d shows that a considerable amount of strain

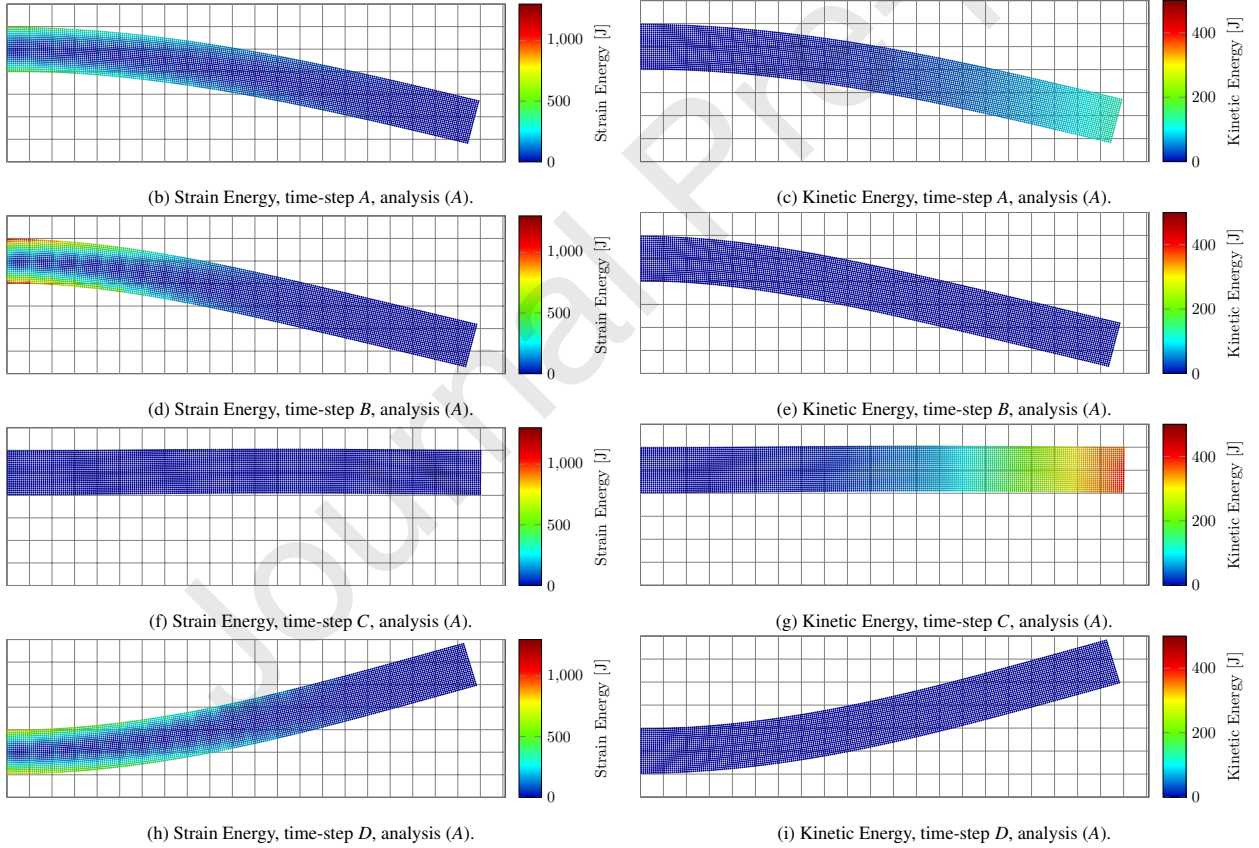
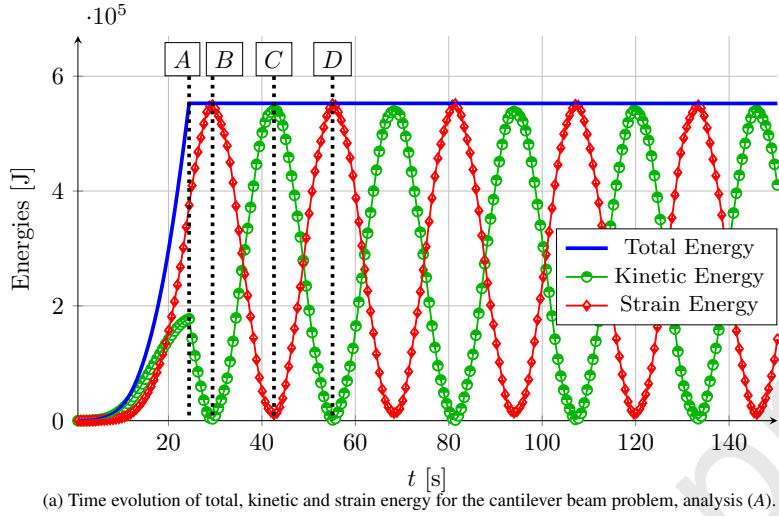
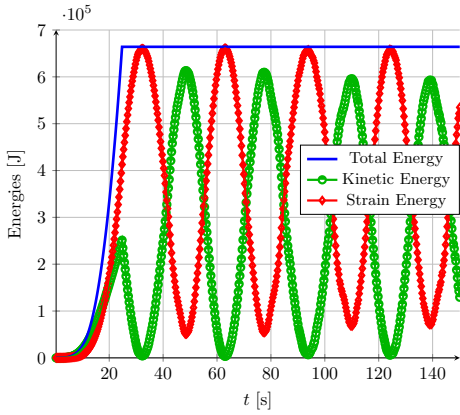
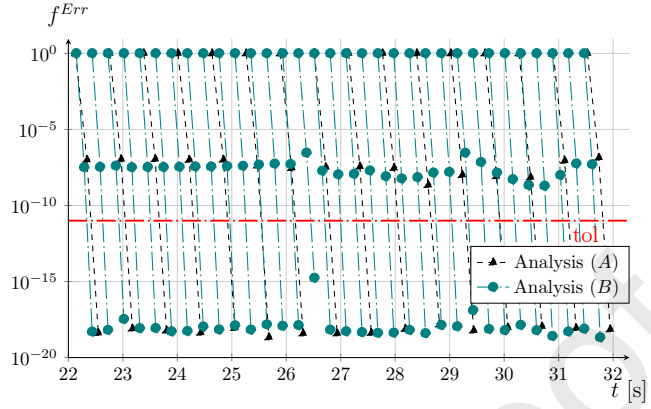


Fig. 4: Time plot of the energies during the simulation (top row) and deflection shapes representing the strain (left) and kinetic (right) energies for time-steps A . . . D. Graphs refer all to analysis (A).



(a) Time evolution of total, kinetic and strain energy for the cantilever beam problem, analysis (B).



(b) Convergence of the Newton-Raphson scheme for time between 22 s and 32 s.

Fig. 5: Time plot of the energies for the simulation (B) (on the left-hand side), and convergence comparison for both the simulations (on the right-hand side).

energy is located at the external fibres in the fixed end. On the other hand, the beam is unstrained in its original configuration at time-step C (Figure 4f), while the kinetic energy (Figure 4g) is distributed with a gradient along the  $x$ -axis, independent of the material points' position along the vertical direction. Time-step D represents another maximum point of the strain energy, with D's deflection shape horizontally mirroring B's. However, when comparing the strain energy of the two configurations (Figure 4h and 4d, respectively), it can be seen how the external fibres in B are more heavily loaded than their respective ones in D. With a closer look, it can be noted how the displacements at the free end of the beam in points B and D do not coincide. This inaccuracy is due to time sampling, which does not accurately capture the peak strain energy. Therefore, points B and D are not temporally spaced as the proper period of the beam would predict. The energies time-response of simulation (B) is plotted in Figure 5a. The structure presents periodic behaviour with a lower frequency time compared to simulation (A). Moreover, it can be seen how the total energy for this simulation is slightly higher than the one for analysis (A), which is due to a higher kinetic energy accumulated in the loading phase for simulation (B).

Figure 5b shows the convergences of the Newton-Raphson algorithm for both the analyses, considering the time-steps from  $\approx 22$  s to  $\approx 32$  s. Even though these steps take difficult passages of the structures into account (time-steps A and B are including in this time interval), it can be seen how the algorithms converge smoothly within three iterations for both the simulations. As highlighted by Coombs and Augarde [29], when dealing with implicit formulations of the MPM, the zeroth iteration is used to build the Jacobian matrix. As such, this iteration was not considered in Figure 5b.

## 7.2. Collision of elastic cylinders

The second example is the collision of two elastic cylinders, and is a common example used in other MPM papers [1; 19; 44; 45]. To model the shape of the cylinders, elements were fully populated by materials points. Materials points lying outside of the given geometry of the cylinders were then discharged. As shown in Table 4,

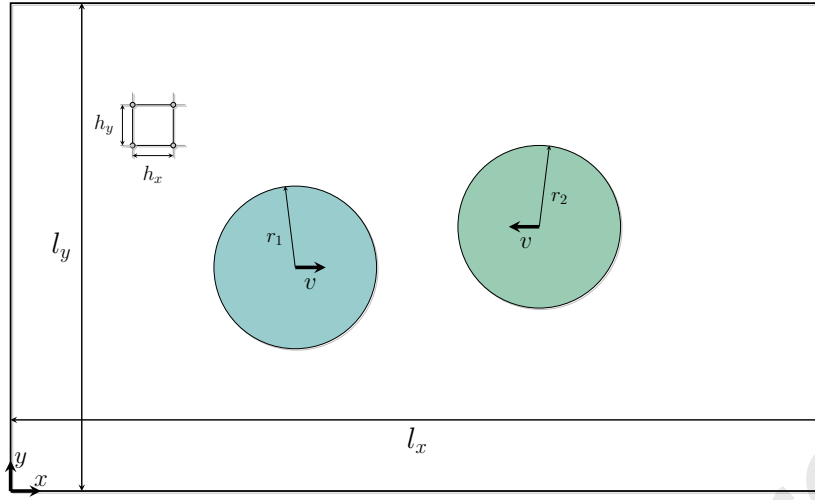


Fig. 6: Illustration of the initial conditions of the cylinder impact problem.

Table 4: Summary of the parameters considered in the analysis of the elastic cylinder collision.

| Parameter Settings               |                                              |                                                    |
|----------------------------------|----------------------------------------------|----------------------------------------------------|
| Material Parameters              | $E_1, E_2$                                   | 100 Pa                                             |
|                                  | $\nu_1, \nu_2$                               | 0.3                                                |
|                                  | $\rho_1, \rho_2$                             | 5 kg/m <sup>3</sup>                                |
| Geometry, Velocities and Timings | $l_x, l_y$                                   | 20, 12 m                                           |
|                                  | $r_1, r_2$                                   | 2 m                                                |
|                                  | $(x_1, y_1), (x_2, y_2)$                     | (5.8, 5.5) m, (14.2, 6.5) m                        |
|                                  | $\ v_1\ , \ v_2\ $                           | 0.75 m/s                                           |
|                                  | $T$                                          | 8 s                                                |
| Analysis Parameters              | $h_x, h_y$                                   | 2 m                                                |
|                                  | $mmp$                                        | 35                                                 |
|                                  | $\Delta t_0, \min(\Delta t), \max(\Delta t)$ | $\approx 0.0573, \approx 0.0562, \approx 0.0655$ s |

the time-step size was not constant during the simulation, but five times the time-step length defined by Eq. (61)<sup>5</sup>, was considered. Nonetheless, the variation of such size is minimal, and this is due to the grid size. As can be seen from Table 4, the grid lengths and number of material points per direction per element ( $mmp$ ) were both significant as this example which could present ill-conditioned mass or Jacobian matrices. This issue is already known from the literature [19] and mainly associated with the poor integration of the above matrices. MPM was used here instead of GIMPM as the small overlap between material points' volume and grid elements' volume is reduced when MPM is applied. Gravity effects were neglected.

Figure 7a shows the time evolution of the energies for four selected time-steps corresponding to  $A \approx 1.89$  s, 32<sup>nd</sup>

<sup>5</sup>Note how running the simulation only five times above the CFL condition is justified by the fact that no numerical dissipation occurs for these simulations within the finite strain context. Hence, these multipliers of the CFL condition cannot be compared with the much larger coefficients used by Guilkey and Weiss [27], as their formulation exhibits numerical damping.

time-step;  $B \approx 2.7$  s,  $45^{th}$  time-step;  $C \approx 3.51$  s,  $58^{th}$  time-step; and  $D \approx 4.9$  s,  $80^{th}$  time-step. In particular,  $A$  and  $C$  correspond to similar levels of energies (both kinetic and strain energy), with the former being more spread on material points (Figures 7c, 7g), and the latter being more concentrated on the material point in the proximity of the nodes where contact between cylinders is taking place (Figures 7b, 7f). However, even if the overall amount of strain and kinetic energies in  $A$  and  $C$  appear to be very similar, these steps present different distributions of energies on material points, as is clear from a comparison of Figures 7b, and 7c for time-step  $A$ , with Figures 7f, and 7g for  $C$ . The minimum kinetic energy (Figure 7e) corresponding to a maximum of the strain energy (Figure 7d) occurs at time-step  $B$ . From this point on, kinetic energy starts to be recovered until time-step  $D$  is reached. This time-step is the end of no-slip contact (computed on the grid, as usual within the MPM framework) between cylinders. As expected from elastic bodies, the deflection shapes of the cylinders (Figures 7h, and 7i) recover circular sections, even though some elastic waves slightly modify them.

### 7.3. Elasto-plastic impact of cylinders

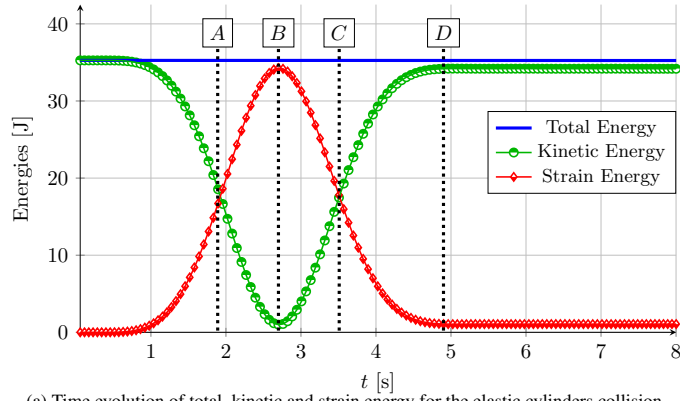
This example is very similar to examples in Meng and Laursen [24], and Love and Sulsky [18]. Even for this case, it has been decided to include two variants: analysis ( $A$ ) (run using the original MPM shape functions) matches the second example above, with the exception that the considered stress-strain relationship is elasto-plastic and the *von Mises* yield function is applied, that is

$$\Phi(\boldsymbol{\tau}) = \frac{\sqrt{2} J_2}{\rho_y} - 1 \leq 0, \quad (62)$$

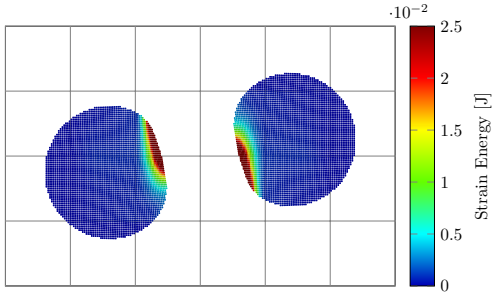
with  $J_2 = \frac{s_{ij} s_{ji}}{2}$ ,  $s_{ij} = \tau_{ij} - \frac{\tau_{kk}}{3} \delta_{ij}$ . On the other hand, analyses ( $B$ ) (run using the GIMPM shape functions) presents a mesh 4 times finer than the one used of ( $A$ ), with  $mmp = 8$ . The parameters that differ from those used in Table 4 are presented below:

- $(\rho_y)_1 = (\rho_y)_2 = 10$  Pa, being the yield stress;
- $\min(\Delta t) \approx 0.0571$  s, and  $\approx 0.06020$  s for analyses ( $A$ ) and ( $B$ ), respectively (being 5 times the minimum time-step size defined by Eq. (61));
- $\max(\Delta t) \approx 0.0666$  s, and  $\approx 0.06023$  s for analyses ( $A$ ) and ( $B$ ), respectively (being 5 times the maximum time-step size defined by Eq. (61));

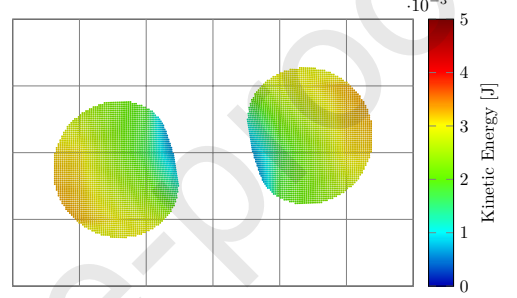
As can be seen from Figure 8a, four time-steps were selected, and their relative deflection shape and energies are represented in Figures 8b-8o:  $A$  at  $\approx 2.9$  s,  $B$  at 3.9 s,  $C$  at 4.4 s, and  $D$  at 6.7 s. From Figure 8a, it can be noticed how the start of the collision, governed by the mesh size and the different stencils of the shape functions, is delayed for simulation ( $B$ ). In this sense, it can be seen how time-step  $A$ , which corresponds to a minimum for the kinetic energy for simulation ( $A$ ) (see Figure 8c), defines instead the initial stages of contact for analysis ( $B$ ) (Figures 8d and 8e). In turn, time-step  $B$  is representative of the same levels of kinetic and strain energies for simulation ( $A$ ) (Figures 8f and 8g), while it is particularly close to the peak of contact for analyses ( $B$ ) (maximum in strain energy, Figure 8h). A second yielding takes place starting from time-step  $C$  and, although with a decreasing trend, continues until the



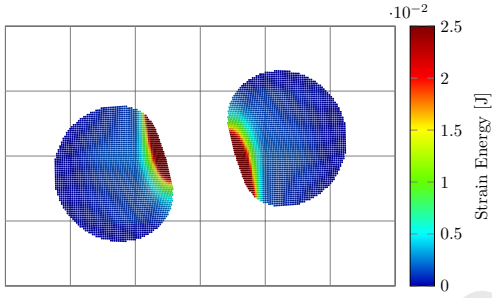
(a) Time evolution of total, kinetic and strain energy for the elastic cylinders collision.



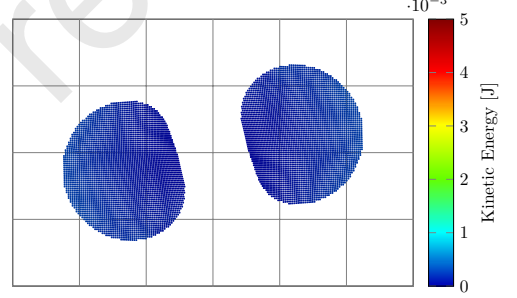
(b) Strain Energy, time-step A.



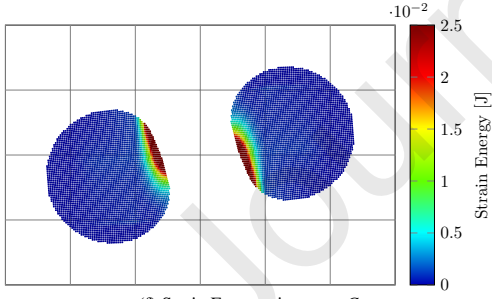
(c) Kinetic Energy, time-step A.



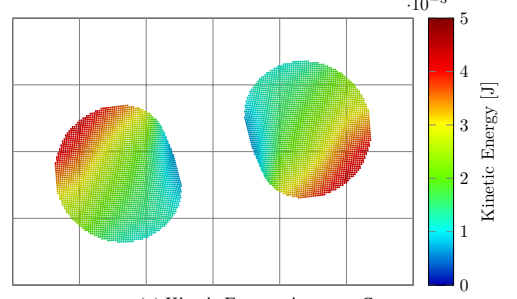
(d) Strain Energy, time-step B.



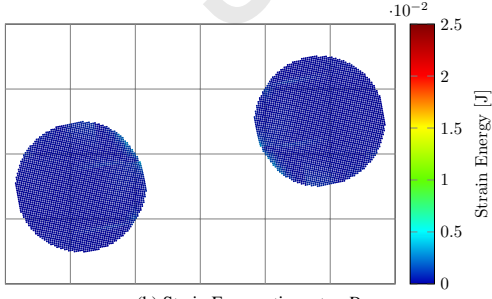
(e) Kinetic Energy, time-step B.



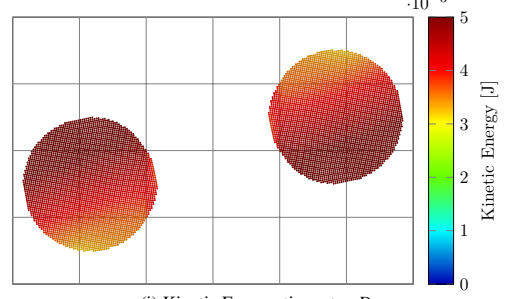
(f) Strain Energy, time-step C.



(g) Kinetic Energy, time-step C.



(h) Strain Energy, time-step D.



(i) Kinetic Energy, time-step D.

Fig. 7: Time plot of the energies during the simulation (top row) and deflection shapes representing the strain (left) and kinetic (right) energies for time-steps A . . . D.

end of the simulation (A). The cause beyond this second yielding can be found in the waves propagating through the bodies after the collision, whose deviatoric part is progressively damped by the von Mises yield function. Time-step  $D$  defines the end of contact for simulation (A) (constant total energy, Figures 8n and 8o), while it can be appreciated from Figures 8p and 8q how contact is still persistent for analysis (B) at this stage.

From a comparison of the strain energies distributions of analysis (A) (Figures 8b, 8f, 8j, and , 8n) with their respective of simulation (B) (Figures 8d, 8h, 8l, and , 8p), it can be noticed how the mesh refinement and the use of different shape functions do not entirely eliminate the dependency of the strain energies from the mesh. From a closer look, it can be appreciated how such strain energy localisations take place in correspondence of element edges or corners. This can be explained with the integration errors discussed in Example 7.1, as material points in correspondence of element boundaries are particularly misplaces from an integration perspective.

#### 7.4. Impact of a Taylor bar

This example considers the classical three-dimensional example of the Taylor bar problem Figure 9, which has been used in the literature as a benchmark for transient dynamic codes both for the FEM [24; 46–49] and for the MPM [18]. The list of parameters necessary to run the analysis is presented in Table 5, and the GIMPM has been considered. The yield function is given by the following equation

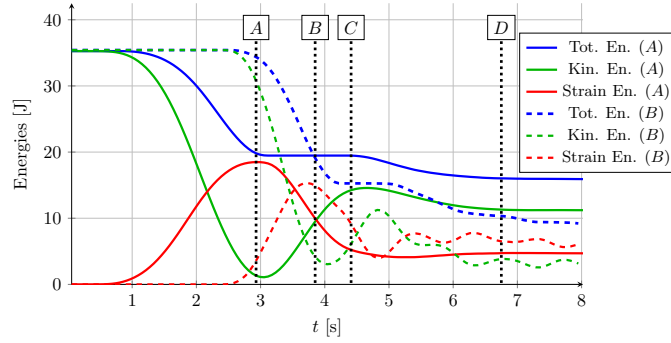
$$\Phi(\tau, q) = \frac{\sqrt{2}J_2}{\sigma_y} - \sqrt{\frac{2}{3}} \left(1 - \frac{q}{\sigma_y}\right) \leq 0, \quad (63)$$

where the values of the yield stress is  $\sigma_y = 0.4$  GPa. The linear hardening parameter is assumed to be  $H = 0.1$  GPa. The time-step length is kept 15 times the value given by Eq. (61). Given the lower number of material points per elements originally chosen, this simulation uses the ghost stabilisation (see, for instance, [41] or [50]) to avoid the integration problem described in 7.1.

The time-history of the energies represented (see Figure 10), the maximum radial and axial displacements (see Figure 11), and the final deflection shape (see Figure 12) are in agreement with those in references [24; 46–49] for the FEM and in [18] for the MPM.

Table 5: Summary of the parameters considered in the analysis of the Taylor bar impact.

| Parameter Settings               |                                              |                                                     |
|----------------------------------|----------------------------------------------|-----------------------------------------------------|
| Material Parameters              | $K, G$                                       | 130, 43.3 GPa                                       |
|                                  | $\rho$                                       | 8930 kg/m <sup>3</sup>                              |
| Geometry, Velocities and Timings | $h_0, r_0$                                   | 32.2, 3.2 mm                                        |
|                                  | $L_x, L_y, L_z$                              | 7.2, 32.2, 7.2 mm                                   |
|                                  | $\ v\  = v_y,$                               | -227 m/s                                            |
|                                  | $T$                                          | 80 $\mu$ s                                          |
| Analysis Parameters              | $h_x, h_y, h_z$                              | 0.8, 0.648, 0.8 mm                                  |
|                                  | $mmp$                                        | 2                                                   |
|                                  | $\Delta t_0, \min(\Delta t), \max(\Delta t)$ | $\approx 0.375, \approx 0.371, \approx 0.375 \mu$ s |



(a) Time evolution of total, kinetic and strain energy for the elasto-plastic cylinders collision.

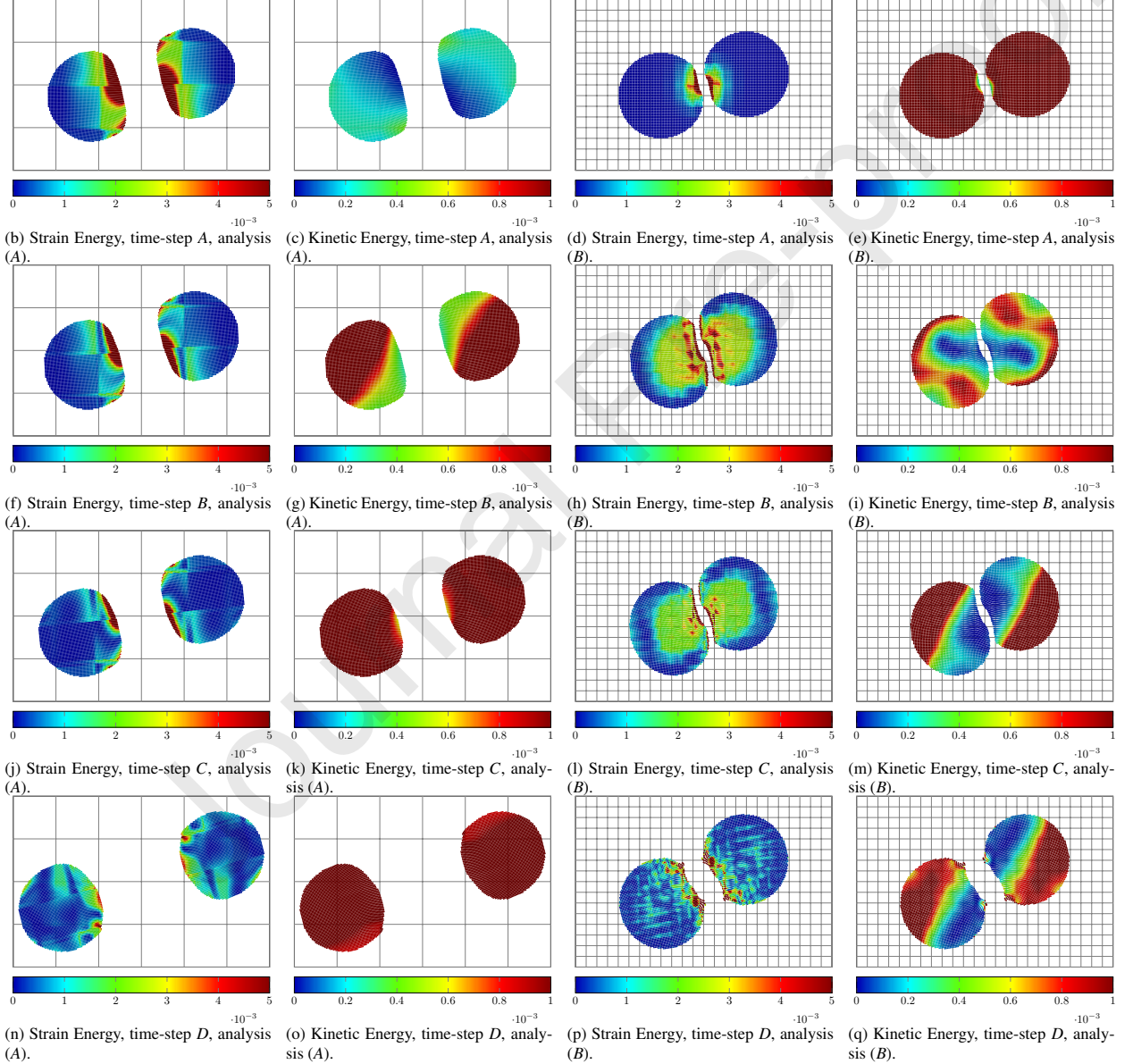


Fig. 8: Time course of the energies during the simulation (top row) and deflection shapes representing the simulation (A) (first two columns) and (B) (last two columns). Strain energy (first and third column) and kinetic energy (second and fourth column) are considered for time-steps A . . . D. Physical dimension of contours are in Joule [J].

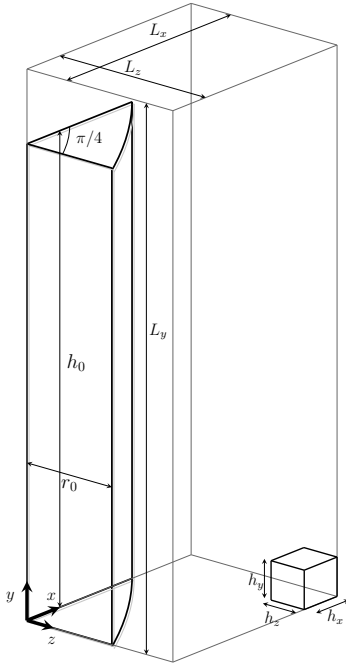


Fig. 9: Illustration of the initial conditions of the Taylor bar problem. Only a quarter of the cylinder has been considered for the analysis.

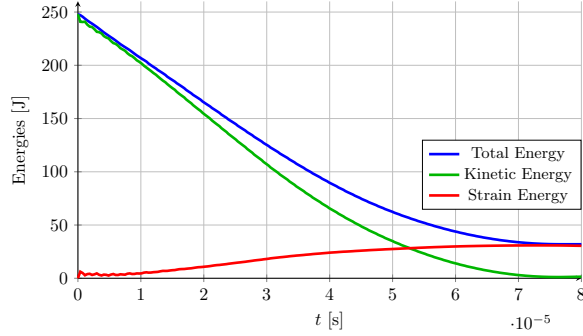


Fig. 10: Time evolution of total, kinetic and strain energy for the elasto-plastic cylinders collision.

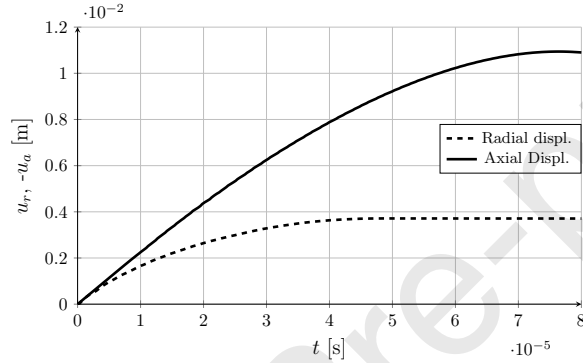


Fig. 11: Displacement history of the maximum radial and axial displacements.

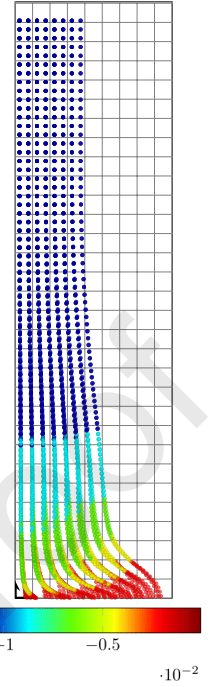


Fig. 12: Deflection shape at the end of the simulation in the  $zy$ -plane. Contours represent the displacement along the  $y$ -direction (expressed in [m]).

## 8. Conclusions and future work

This paper extends the MPM to an updated Lagrangian formulation in the context of the isotropic multiplicative elasto-plastic theory. Two mapping procedures are assessed, and new light is shed on the connection between the material point-to-grid and grid-to-material point mappings in the case of deformable body dynamics. In addition, the presence of non-linearity requires careful choice of time-step size and it has been shown that the CFL condition can be used as a useful tool in setting the time step size for practical analyses. The standard approach of setting a constant time step size for a given analysis is problematic for the MPM as it requires the estimation of the *worst* case (the smallest time step size required for a given time step) *a priori*, which is almost impossible due to the evolving nature of the distribution of mass and stiffness within discretised governing equations during an analysis. The CFL-based adaptive approach proposed in this paper has the potential to improve the adaptivity of the time-step size for the implicit material point method.

It should be emphasised that the formulation is very convenient for low-frequency problems, whose time duration, especially when extended, is ensured by maintaining the properties inherited from the continuous formulation and guaranteed by proper mapping procedures and compliant modifications of the constitutive relation. However, ongoing studies show that the current method performs well for high-frequency problems, with the caveat that the time-step length should be changed to no more than one order of magnitude above the value defined by Eq. (61). In this fashion, the wave oscillating through the medium are entirely reproduced by this technique.

This method can additionally be used as a basis for validating other features which can be implemented in the MPM from an energy perspective, such as frictional contact, within the finite strain theory.

To further extend the convenience of the proposed algorithm, further work would be valuable to locate techniques to invert the mass matrix and the Jacobian matrix without incurring numerical errors. To avoid such errors, the proposed method resorted to the use of a higher number of integration points for the Examples 7.1-7.3. However, the stabilisation employed in the Example 7.4 proves that, when a lower number of integration points is considered, techniques to improve the algorithm's stability are necessary. The assessment of these methods under a conservation laws perspective will be part of further studies. Another natural extension of the algorithm would be the modelling of multi-phase materials. Such a method would have to be ascertained in terms of conservation properties for both the mappings and constitutive relationships, in the same way as proposed here for a deformable solid body.

A different interesting extension to the current model could consist in considering anisotropic behaviour, especially given that MPM has been used to model wood (see [51; 52]), which exhibits orthotropic behaviour.

## Acknowledgements

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## Appendix A. Linearisation

### Appendix A.1. Linearisation of the internal force vector

The internal force vector defined by Eq. (44) can be expressed in index notation as

$$(\mathbf{f}_\theta^{\text{int}})_I = \int_{\Omega_0} (\nabla_{x_r} \mathbf{N})_{Ip} (\Delta F_{\Delta t - \theta}^{-1})_{pq} \tau_{qr}^{mp} dV_0. \quad (\text{A.1})$$

The linearisation of the above quantity with respect to the nodal displacements evaluated at the end of the time-step is the so-called *stiffness matrix*  $\mathbf{K}_{IJ}$ , and it is useful to express it by using the following chain rule

$$\begin{aligned} \mathbf{K}_{IJ} &= \frac{\partial (\mathbf{f}_\theta^{\text{int}})_I}{\partial (\mathbf{u}_{n+1})_J} = \int_{\Omega_0} \left( \frac{\partial (\bullet)_I}{\partial (F)_{mn}} \frac{\partial (F)_{mn}}{\partial (\mathbf{u}_{n+1})_J} \right) dV_0 = \int_{\Omega_0} \left( \frac{\partial (\bullet)_I}{\partial (F)_{mn}} \frac{\partial}{\partial (\mathbf{u}_{n+1})_J} \left( \frac{\partial x_m}{\partial X_n} \right) \right) dV_0 = \\ &= \int_{\Omega_0} \left( \frac{\partial (\bullet)_I}{\partial (F)_{mn}} \frac{\partial}{\partial (\mathbf{u}_{n+1})_J} \left( \delta_{mn} + \frac{\partial \mathbf{N}_{mH} (\mathbf{u}_{n+1})_H}{\partial X_n} \right) \right) dV_0 = \int_{\Omega_0} \left( \frac{\partial (\bullet)_I}{\partial (F)_{mn}} \frac{\partial \mathbf{N}_{mH} \delta_{HJ}}{\partial X_n} \right) dV_0 = \\ &= \int_{\Omega_0} \left( \frac{\partial (\bullet)_I}{\partial (F)_{mn}} \nabla_{x_s} \mathbf{N}_{mJ} F_{sn} \right) dV_0. \end{aligned} \quad (\text{A.2})$$

By using Eq. (A.2), the stiffness matrix can be expressed as

$$\begin{aligned}
K_{IJ} = & \int_{\Omega_{t+\Delta t}} \left( \frac{1}{J} \frac{\partial}{\partial F_{mn}} \left( \frac{\partial N_{Ip}}{\partial x_r} \right) (\Delta F_{\Delta t-\theta}^{-1})_{pq} \tau_{qr}^{mp} \nabla_{x_s} N_{mJ} F_{sn} + \frac{1}{J} \nabla_{x_r} N_{Ip} \frac{\partial (\Delta F_{\Delta t-\theta}^{-1})_{pq}}{\partial F_{mn}} \tau_{qr}^{mp} \nabla_{x_s} N_{mJ} F_{sn} \right. \\
& \left. + \frac{1}{J} \nabla_{x_r} N_{Ip} (\Delta F_{\Delta t-\theta}^{-1})_{pq} \frac{\partial \tau_{qr}^{mp}}{\partial F_{mn}} \nabla_{x_s} N_{mJ} F_{sn} \right) dV_{t+\Delta t} \\
= & \int_{\Omega_{t+\Delta t}} \left( \frac{1}{J} \frac{\partial N_{Ip}}{\partial X_u} \frac{\partial (F^{-1})_{ur}}{\partial F_{mn}} (\Delta F_{\Delta t-\theta}^{-1})_{pq} \tau_{qr}^{mp} \nabla_{x_s} N_{mJ} F_{sn} + \frac{1}{J} \nabla_{x_r} N_{Ip} \frac{\partial (\Delta F_{\Delta t-\theta}^{-1})_{pq}}{\partial F_{mn}} \tau_{qr}^{mp} \nabla_{x_s} N_{mJ} F_{sn} \right. \\
& \left. + \frac{1}{J} \nabla_{x_r} N_{Ip} (\Delta F_{\Delta t-\theta}^{-1})_{pq} \frac{\partial \tau_{qr}^{mp}}{\partial F_{mn}} \nabla_{x_s} N_{mJ} F_{sn} \right) dV_{t+\Delta t}. \quad (A.3)
\end{aligned}$$

467

468 To proceed with the linearisation process, it is convenient to re-write the quantity  $\Delta F_{\Delta t-\theta}^{-1}$  as

$$\begin{aligned}
\Delta F_{\Delta t-\theta}^{-1} &= \frac{\partial \mathbf{x}_\theta}{\partial \mathbf{X}} \frac{\partial \mathbf{X}}{\partial \mathbf{x}} = \frac{\partial}{\partial \mathbf{X}} (\tilde{\mathbf{X}} + \vartheta \Delta \mathbf{u}) \frac{\partial \mathbf{X}}{\partial \mathbf{x}} = \frac{\partial}{\partial \mathbf{X}} ((1-\vartheta) \tilde{\mathbf{X}} + \vartheta \mathbf{x}) \frac{\partial \mathbf{X}}{\partial \mathbf{x}} \\
&= ((1-\vartheta) \mathbf{F}_t + \vartheta \mathbf{F}) \mathbf{F}^{-1} = (1-\vartheta) \Delta \mathbf{F}^{-1} + \vartheta \mathbf{I}^{(2)}, \quad (A.4)
\end{aligned}$$

469 with  $\mathbf{I}^{(2)}$  being the second-order identity tensor, i.e.  $\mathbf{I}^{(2)} = \delta_{ij}$ . Hence, the linearisation of the above quantity is  
 470 straightforward and, in the case where  $\vartheta = \frac{1}{2}$  (as assumed for the mid-point rule), its derivative becomes

$$\frac{\partial (\Delta F_{\Delta t-1/2}^{-1})_{pq}}{\partial F_{mn}} = \frac{1}{2} \frac{\partial}{\partial F_{mn}} \left( (F_t)_{p\alpha} (F^{-1})_{\alpha q} + \delta_{pq} \right) = -\frac{1}{2} (F_t)_{p\alpha} (F^{-1})_{\alpha m} (F^{-1})_{nq}.$$

471 Therefore, Eq. (A.3) can be written as

$$\begin{aligned}
K_{IJ} = & \int_{\Omega_{t+\Delta t}} \left( -\frac{1}{J} \nabla_{x_m} N_{Ip} (\Delta F_{\Delta t-\theta}^{-1})_{pq} \tau_{qr}^{mp} \delta_{rs} \nabla_{x_s} N_{mJ} - \frac{1}{2J} \nabla_{x_r} N_{Ip} \tau_{qr}^{mp} (\Delta F^{-1})_{pm} \delta_{qs} \nabla_{x_s} N_{mJ} \right. \\
& \left. + \frac{1}{J} \nabla_{x_r} N_{Ip} (\Delta F_{\Delta t-\theta}^{-1})_{pq} \frac{\partial \tau_{qr}^{mp}}{\partial F_{mn}} \nabla_{x_s} N_{mJ} F_{sn} \right) dV_{t+\Delta t}. \quad (A.5)
\end{aligned}$$

472 It is also useful to gather the stress quantity  $\Delta F_{\Delta t-\theta}^{-1} \tau^{mp}$  as a unique asymmetric tensor, which is defined as

$$\check{P}_{pr} = (\Delta F_{\Delta t-\theta}^{-1})_{pq} \tau_{qr}^{mp}. \quad (A.6)$$

473 Moreover, the first term can be written as

$$\begin{aligned}
\frac{\partial N_{Ip}}{\partial x_m} \check{P}_{pr} \delta_{rs} \frac{\partial N_{mJ}}{\partial x_s} &= \frac{\partial N_{Ip}}{\partial x_m} \check{P}_{ps} \frac{\partial N_{mJ}}{\partial x_s} \\
&= \frac{\partial N_{Ip}}{\partial x_r} \check{P}_{ps} \delta_{rm} \frac{\partial N_{mJ}}{\partial x_s}. \quad (A.7)
\end{aligned}$$

474 Owing to the above equations, the *stiffness matrix* becomes

$$K_{IJ} = \int_{\Omega_{t+\Delta t}} \left( -\frac{1}{J} \nabla_{x_r} N_{Ip} \check{P}_{ps} \delta_{rm} \nabla_{x_s} N_{mJ} - \frac{1}{2J} \nabla_{x_r} N_{Ip} \tau_{sr}^{mp} (\Delta F^{-1})_{pm} \nabla_{x_s} N_{mJ} \right) dV_{t+\Delta t}$$

$$+ \frac{1}{J} \nabla_{x_r} N_{Ip} \left( \Delta F_{\Delta t - \theta}^{-1} \right)_{pq} \frac{\partial \tau_{qr}^{mp}}{\partial F_{mn}} \nabla_{x_s} N_{mJ} F_{sn} \Big) dV_{t+\Delta t}. \quad (\text{A.8})$$

The terms in the above equation can be collected in the so-called *spatial tangent modulus*  $\check{\alpha}_{prms}$  as follows

$$\check{\alpha}_{prms} := \underbrace{-\frac{1}{J} \check{P}_{ps} \delta_{rm}}_{:=\mathcal{P}_{prms}} - \underbrace{\frac{1}{2J} \tau_{sr}^{mp} \left( \Delta F^{-1} \right)_{pm}}_{:=\Theta_{prms}} + \frac{1}{J} \left( \Delta F_{\Delta t - \theta}^{-1} \right)_{pq} \frac{\partial \tau_{qr}^{mp}}{\partial F_{mn}} F_{sn}. \quad (\text{A.9})$$

Therefore, the stiffness matrix can be concisely expressed as

$$K_{IJ} = \int_{\Omega_{t+\Delta t}} \nabla_{x_r} N_{Ip} \check{\alpha}_{prms} \nabla_{x_s} N_{mJ} dV_{t+\Delta t}. \quad (\text{A.10})$$

It can be noticed that the first and last components of the fourth-order tensor  $\check{\alpha}_{prms}$  in Eq. (A.9) are the classical linearised terms which have to be computed in an updated Lagrangian formulation (see, for a comparison, de Souza Neto *et al.* [38]). The second additional term is due to the misalignment between the (intermediate) configuration where the equilibrium is imposed and the (current) configuration where the algorithmic Kirchhoff stress has been mapped.

#### Appendix A.2. Linearisation of the algorithmic Kirchhoff stress

Owing to the definition of  $\tau^{mp}$  given in Eq. (51), the derivative of such quantity with respect to the deformation gradient is as follows:

$$\begin{aligned} \frac{\partial \tau_{qr}^{mp}}{\partial F_{mn}} &= \frac{\partial}{\partial F_{mn}} \left( \bar{\tau}_{qr} + \Delta^{PF} b_{qr} \left( \frac{\Delta \mathcal{H}^{int}}{\|\Delta C\|^2} \right) \right) \\ &= \frac{\partial \bar{\tau}_{qr}}{\partial F_{mn}} + \frac{\partial \Delta^{PF} b_{qr}}{\partial F_{mn}} \left( \frac{\Delta \mathcal{H}^{int}}{\|\Delta C\|^2} \right) + \frac{\Delta^{PF} b_{qr}}{\|\Delta C\|^4} \left( \frac{\partial \Delta \mathcal{H}^{int}}{\partial F_{mn}} \|\Delta C\|^2 - \Delta \mathcal{H}^{int} \frac{\partial \|\Delta C\|^2}{\partial F_{mn}} \right). \end{aligned} \quad (\text{A.11})$$

The derivatives of the quantities in the above equation can be evaluated in this way:

$$\begin{aligned} \frac{\partial \bar{\tau}_{qr}}{\partial F_{mn}} &= \frac{1}{2} \frac{\partial}{\partial F_{mn}} \left( \Delta F_{q\alpha} (\tau_t)_{\alpha\beta} \Delta F_{r\beta} + (\tau_{t+\Delta t})_{qr} \right) \\ &= \frac{1}{2} \left( \delta_{qm} \left( F_t^{-1} \right)_{n\alpha} (\tau_t)_{\alpha\beta} \Delta F_{r\beta} + \Delta F_{q\alpha} (\tau_t)_{\alpha\beta} \delta_{rm} \left( F_t^{-1} \right)_{n\beta} + \frac{\partial (\tau_{t+\Delta t})_{qr}}{\partial F_{mn}} \right); \end{aligned} \quad (\text{A.12})$$

$$\begin{aligned} \frac{\partial \Delta^{PF} b_{qr}}{\partial F_{mn}} &= \frac{\partial}{\partial F_{mn}} \left( F_{q\alpha} F_{\gamma\alpha} F_{\gamma\beta} F_{r\beta} - F_{q\alpha} (F_t)_{\gamma\alpha} (F_t)_{\gamma\beta} F_{r\beta} \right) \\ &= \delta_{qm} (\Delta C)_{n\beta} F_{r\beta} + F_{q\alpha} (\Delta C)_{\alpha n} \delta_{rm} + F_{qn} F_{m\beta} F_{r\beta} + F_{q\alpha} F_{m\alpha} F_{rn}; \end{aligned} \quad (\text{A.13})$$

$$\frac{\partial \|\Delta C\|^2}{\partial F_{mn}} = \frac{\partial}{\partial F_{mn}} \left( (\Delta C)_{\alpha\beta} (\Delta C)_{\alpha\beta} \right) = 2 \left( F_{m\beta} \Delta C_{n\beta} + F_{m\alpha} \Delta C_{\alpha n} \right);$$

$$\frac{\partial \Delta \mathcal{H}^{int}}{\partial F_{mn}} = \frac{\partial}{\partial F_{mn}} \left( 2 \left( \Delta \psi + \Delta \mathcal{D}^{int} \right) - 2 \bar{\tau}_{\delta\epsilon} \bar{d}_{\delta\epsilon} \right) = 2 \frac{\partial \Delta \psi}{\partial F_{mn}} + 2 \frac{\partial \Delta \mathcal{D}^{int}}{\partial F_{mn}} - 2 \left( \frac{\partial \bar{\tau}_{\delta\epsilon}}{\partial F_{mn}} \bar{d}_{\delta\epsilon} + \frac{\partial \bar{d}_{\delta\epsilon}}{\partial F_{mn}} \bar{\tau}_{\delta\epsilon} \right).$$

489 To evaluate the derivative of the strain energy, it is necessary to introduce the kind of material we are considering. In  
 490 this case, we take a Hencky material into account with isotropic hardening, whose strain energy function is defined  
 491 by  $\psi = \underbrace{\frac{1}{2} \epsilon^e \mathcal{D}^e \epsilon^e}_{\psi^e(\epsilon^e)} + \underbrace{\frac{1}{2} H \xi^2}_{\psi^p(\xi)}$  (with  $H \geq 0$  being the hardening parameter). Hence, it follows that

$$\begin{aligned} \frac{\partial \Delta \psi}{\partial F_{mn}} &= \frac{\partial \psi(\epsilon_{t+\Delta t}^e, \xi_{t+\Delta t})}{\partial F_{mn}} = \frac{\partial \psi^e(\epsilon_{t+\Delta t}^e)}{\partial (\epsilon_{t+\Delta t}^e)_{cd}} \frac{\partial (\epsilon_{t+\Delta t}^e)_{cd}}{\partial (\tau_{t+\Delta t})_{ab}} \frac{\partial (\tau_{t+\Delta t})_{ab}}{\partial F_{mn}} + \frac{\partial \psi^p(\xi_{t+\Delta t})}{\partial \xi_{t+\Delta t}} \frac{\partial \xi_{t+\Delta t}}{\partial q_{t+\Delta t}} \frac{\partial q_{t+\Delta t}}{\partial F_{mn}} = \\ &= (\epsilon_{t+\Delta t}^e)_{ab} \frac{\partial (\tau_{t+\Delta t})_{ab}}{\partial F_{mn}} - \xi_{t+\Delta t} \frac{\partial q_{t+\Delta t}}{\partial F_{mn}}. \end{aligned} \quad (\text{A.14})$$

492 On the other hand, the derivative of the internal dissipation  $\Delta \mathcal{D}^{int}$  is a function of the yield function  $\Phi$ . In this case,  
 493 we do not specify any yield function, so that the derivatives are the most general ones<sup>6</sup>:

$$\begin{aligned} \frac{\partial \Delta \mathcal{D}^{int}}{\partial F_{mn}} &= \frac{\partial \Delta \mathcal{D}^{int}}{\partial (\epsilon_{t+\Delta t}^{e,trial})_{hk}} \frac{\partial (\epsilon_{t+\Delta t}^{e,trial})_{hk}}{\partial F_{mn}} \\ &= \frac{\partial}{\partial (\epsilon_{t+\Delta t}^{e,trial})_{hk}} \left( \Delta \gamma (\tau_{t+\Delta t})_{\alpha\beta} \frac{\partial \Phi}{\partial (\tau_{t+\Delta t})_{\alpha\beta}} + \Delta \gamma q_{t+\Delta t} \frac{\partial \Phi}{\partial q_{t+\Delta t}} \right) \frac{\partial (\epsilon_{t+\Delta t}^{e,trial})_{hk}}{\partial F_{mn}} \\ &= \left( \frac{\partial \Delta \gamma}{\partial (\epsilon_{t+\Delta t}^{e,trial})_{hk}} \left( (\tau_{t+\Delta t})_{\alpha\beta} \frac{\partial \Phi}{\partial (\tau_{t+\Delta t})_{\alpha\beta}} + q_{t+\Delta t} \frac{\partial \Phi}{\partial q_{t+\Delta t}} \right) + \Delta \gamma I_{\alpha\beta ab}^{4,sym} \frac{\partial (\tau_{t+\Delta t})_{ab}}{\partial (\epsilon_{t+\Delta t}^{e,trial})_{hk}} \left( \frac{\partial \Phi}{\partial (\tau_{t+\Delta t})_{\alpha\beta}} \right) \right. \\ &\quad + \Delta \gamma (\tau_{t+\Delta t})_{\alpha\beta} \left( \frac{\partial}{\partial (\tau_{t+\Delta t})_{ab}} \left( \frac{\partial \Phi}{\partial (\tau_{t+\Delta t})_{\alpha\beta}} \right) \frac{\partial (\tau_{t+\Delta t})_{ab}}{\partial (\epsilon_{t+\Delta t}^{e,trial})_{hk}} + \frac{\partial}{\partial q_{t+\Delta t}} \left( \frac{\partial \Phi}{\partial (\tau_{t+\Delta t})_{\alpha\beta}} \right) \frac{\partial q_{t+\Delta t}}{\partial (\epsilon_{t+\Delta t}^{e,trial})_{hk}} \right) \\ &\quad \left. + \Delta \gamma \left( \frac{\partial q_{t+\Delta t}}{\partial (\epsilon_{t+\Delta t}^{e,trial})_{hk}} \frac{\partial \Phi}{\partial q_{t+\Delta t}} + q_{t+\Delta t} \left( \frac{\partial}{\partial (\tau_{t+\Delta t})_{ab}} \left( \frac{\partial \Phi}{\partial q_{t+\Delta t}} \right) \frac{\partial (\tau_{t+\Delta t})_{ab}}{\partial (\epsilon_{t+\Delta t}^{e,trial})_{hk}} + \frac{\partial^2 \Phi}{(\partial q_{t+\Delta t})^2} \frac{\partial q_{t+\Delta t}}{\partial (\epsilon_{t+\Delta t}^{e,trial})_{hk}} \right) \right) \right) \frac{\partial (\epsilon_{t+\Delta t}^{e,trial})_{hk}}{\partial F_{mn}} \\ &= \left( (\partial \Delta \mathcal{D}^{int})_{(1)}^{int} \right)_{hk} + \left( (\partial \Delta \mathcal{D}^{int})_{(2)}^{int} \right)_{ab} \frac{\partial (\tau_{t+\Delta t})_{ab}}{\partial (\epsilon_{t+\Delta t}^{e,trial})_{hk}} \frac{\partial (\epsilon_{t+\Delta t}^{e,trial})_{hk}}{\partial F_{mn}}, \end{aligned} \quad (\text{A.15})$$

494 where the quantities  $(\partial \Delta \mathcal{D}^{int})_{(1)}^{int}$  and  $(\partial \Delta \mathcal{D}^{int})_{(2)}^{int}$  have been defined as

$$\begin{aligned} (\partial \Delta \mathcal{D}^{int})_{(1)}^{int} &:= \frac{\partial \Delta \gamma}{\partial (\epsilon_{t+\Delta t}^{e,trial})_{hk}} \left( (\tau_{t+\Delta t})_{\alpha\beta} \frac{\partial \Phi}{\partial (\tau_{t+\Delta t})_{\alpha\beta}} + q_{t+\Delta t} \frac{\partial \Phi}{\partial q_{t+\Delta t}} \right) \\ &\quad + \Delta \gamma \frac{\partial q_{t+\Delta t}}{\partial (\epsilon_{t+\Delta t}^{e,trial})_{hk}} \left( (\tau_{t+\Delta t})_{\alpha\beta} \frac{\partial}{\partial q_{t+\Delta t}} \left( \frac{\partial \Phi}{\partial (\tau_{t+\Delta t})_{\alpha\beta}} \right) + \frac{\partial \Phi}{\partial q_{t+\Delta t}} + q_{t+\Delta t} \frac{\partial^2 \Phi}{(\partial q_{t+\Delta t})^2} \right); \end{aligned} \quad (\text{A.16})$$

$$(\partial \Delta \mathcal{D}^{int})_{(2)}^{int} := \Delta \gamma \left( \frac{\partial \Phi}{\partial (\tau_{t+\Delta t})_{ab}} + (\tau_{t+\Delta t})_{\alpha\beta} \frac{\partial^2 \Phi}{\partial (\tau_{t+\Delta t})_{ab} \partial (\tau_{t+\Delta t})_{\alpha\beta}} + q_{t+\Delta t} \frac{\partial}{\partial (\tau_{t+\Delta t})_{ab}} \left( \frac{\partial \Phi}{\partial q_{t+\Delta t}} \right) \right), \quad (\text{A.17})$$

495 and  $I_{\alpha\beta ab}^{4,sym} = \frac{1}{2} (\delta_{\alpha\alpha} \delta_{\beta\beta} + \delta_{\alpha\beta} \delta_{\beta\alpha})$  is the fourth-order symmetric identity tensor. In the above equations, the first and  
 496 second derivatives of the yield function and the derivative of the plastic multiplier and of the hardening variable with  
 497 respect to the logarithmic trial elastic strain need to be additionally computed since they have been already evaluated  
 498 for the Jacobian matrix and its inverse in the classical elasto-plastic subroutine (for details, see de Souza Neto [38],  
 499 for instance). Moreover, due to the chosen yield function, it can be seen that  $\frac{\partial^2 \Phi}{(\partial q_{t+\Delta t})^2} = 0$  and  $\frac{\partial}{\partial \tau_{t+\Delta t}} \left( \frac{\partial \Phi}{\partial \tau_{t+\Delta t}} \right) : \tau_{t+\Delta t} =$

<sup>6</sup>Nonetheless, the hardening parameter  $q$  is neglected since this term would add no further mathematical complexity to the considered problem.

$$\frac{\partial}{\partial \tau_{t+\Delta t}} \left( \frac{\partial \Phi}{\partial q_{t+\Delta t}} \right) = \mathbf{0}.$$

The other derivatives in Eq. (A.14) are

$$\begin{aligned} \frac{\partial \bar{\tau}_{\delta\epsilon}}{\partial F_{mn}} \bar{d}_{\delta\epsilon} &= \frac{1}{2} \left( \delta_{\delta m} (F_t^{-1})_{n\alpha} (\tau_t)_{\alpha\beta} \Delta F_{\epsilon\beta} + \Delta F_{\delta\alpha} (\tau_t)_{\alpha\beta} \delta_{\epsilon m} (F_t^{-1})_{n\beta} + \frac{\partial (\tau_{t+\Delta t})_{\delta\epsilon}}{\partial F_{mn}} \right) \bar{d}_{\delta\epsilon} \\ &= \frac{1}{2} \left( (F_t^{-1})_{n\alpha} (\tau_t)_{\alpha\beta} \Delta F_{\epsilon\beta} \bar{d}_{m\epsilon} + \Delta F_{\delta\alpha} (\tau_t)_{\alpha\beta} (F_t^{-1})_{n\beta} \bar{d}_{\delta m} + \frac{\partial (\tau_{t+\Delta t})_{\delta\epsilon}}{\partial F_{mn}} \bar{d}_{\delta\epsilon} \right); \end{aligned} \quad (\text{A.18})$$

$$\frac{\partial \bar{d}_{\delta\epsilon}}{\partial F_{mn}} \bar{\tau}_{\delta\epsilon} = \bar{\tau}_{\delta\epsilon} \frac{\partial}{\partial F_{mn}} \left( \frac{1}{2} (\delta_{\delta\epsilon} - \Delta F_{\alpha\delta}^{-1} \Delta F_{\alpha\epsilon}^{-1}) \right) \quad (\text{A.19})$$

$$= \frac{1}{2} \bar{\tau}_{\delta\epsilon} \left( (\Delta F^{-1})_{\alpha m} (F^{-1})_{n\delta} (\Delta F^{-1})_{\alpha\epsilon} + (\Delta F^{-1})_{\alpha\delta} (\Delta F^{-1})_{\alpha m} (F^{-1})_{n\epsilon} \right). \quad (\text{A.20})$$

To collect the derivatives of the Kirchhoff stress evaluated at the end of the step with respect to the deformation gradient, the following index desaturations are necessary in Eq. (A.18)

$$\frac{\partial (\tau_{t+\Delta t})_{\delta\epsilon}}{\partial F_{mn}} \bar{d}_{\delta\epsilon} = \bar{d}_{\delta\epsilon} I_{\delta\epsilon ab}^{4,\text{sym}} \frac{\partial (\tau_{t+\Delta t})_{ab}}{\partial F_{mn}} = \bar{d}_{ab} \frac{\partial (\tau_{t+\Delta t})_{ab}}{\partial F_{mn}}, \quad (\text{A.21})$$

where the unsolved derivative  $\frac{\partial (\tau_{t+\Delta t})_{ab}}{\partial F_{mn}}$  can be classically developed via the chain rule (see, for instance, de Souza Neto *et al.* [38]) as follows

$$\frac{\partial (\tau_{t+\Delta t})_{ab}}{\partial F_{mn}} = \frac{\partial (\tau_{t+\Delta t})_{ab}}{\partial (\epsilon_{t+\Delta t}^{e,\text{trial}})_{hk}} \frac{\partial (\epsilon_{t+\Delta t}^{e,\text{trial}})_{hk}}{\partial (b_{t+\Delta t}^{e,\text{trial}})_{lu}} \frac{\partial (b_{t+\Delta t}^{e,\text{trial}})_{lu}}{\partial F_{mn}}. \quad (\text{A.22})$$

Hence, it is useful to collect the terms in Eq. (A.11) in this fashion

$$\frac{\partial \tau_{qr}^{mp}}{\partial F_{mn}} = \mathcal{G}_{qrmn} + \left( \mathcal{F}_{qrab} \frac{\partial (\tau_{t+\Delta t})_{ab}}{\partial (\epsilon_{t+\Delta t}^{e,\text{trial}})_{hk}} + \mathcal{H}_{qrhk} \right) \frac{\partial (\epsilon_{t+\Delta t}^{e,\text{trial}})_{hk}}{\partial F_{mn}}, \quad (\text{A.23})$$

where the fourth-order tensors  $\mathcal{G}_{qrmn}$ ,  $\mathcal{F}_{qrab}$  and  $\mathcal{H}_{qrhk}$  have been defined as

$$\begin{aligned} \mathcal{G}_{qrmn} &:= \frac{1}{2} \left( \delta_{qm} (F_t^{-1})_{n\alpha} (\tau_t)_{\alpha\beta} \Delta F_{r\beta} + \Delta F_{q\alpha} (\tau_t)_{\alpha\beta} \delta_{rm} (F_t^{-1})_{n\beta} \right) \\ &\quad + \frac{\Delta \mathcal{H}^{\text{int}}}{\|\Delta \mathbf{C}\|^2} \left( \delta_{qm} (\Delta \mathbf{C})_{n\beta} F_{r\beta} + F_{q\alpha} (\Delta \mathbf{C})_{\alpha n} \delta_{rm} + F_{qn} F_{m\beta} F_{r\beta} + F_{q\alpha} F_{m\alpha} F_{rn} \right) \\ &\quad - \frac{1}{\|\Delta \mathbf{C}\|^2} \Delta^{PF} b_{qr} \left( (F_t^{-1})_{n\alpha} (\tau_t)_{\alpha\beta} \Delta F_{\epsilon\beta} \bar{d}_{m\epsilon} + \Delta F_{\delta\alpha} (\tau_t)_{\alpha\beta} (F_t^{-1})_{n\beta} \bar{d}_{\delta m} \right. \\ &\quad \left. + \bar{\tau}_{\delta\epsilon} (\Delta F^{-1})_{\alpha m} (F^{-1})_{n\delta} (\Delta F^{-1})_{\alpha\epsilon} + \bar{\tau}_{\delta\epsilon} (\Delta F^{-1})_{\alpha\delta} (\Delta F^{-1})_{\alpha m} (F^{-1})_{n\epsilon} \right. \\ &\quad \left. + 2 \frac{\Delta \mathcal{H}^{\text{int}}}{\|\Delta \mathbf{C}\|^2} (F_{m\beta} \Delta C_{n\beta} + F_{m\alpha} \Delta C_{\alpha n}) \right); \end{aligned} \quad (\text{A.24})$$

$$\mathcal{F}_{qrab} := \frac{1}{2} I_{qrab}^{4,\text{sym}} + \frac{1}{\|\Delta \mathbf{C}\|^2} \Delta^{PF} b_{qr} \left( 2 (\epsilon_{t+\Delta t}^e)_{ab} + 2 (\partial \Delta \mathcal{D}_{(2)}^{\text{int}})_{ab} - \bar{d}_{ab} \right); \quad (\text{A.25})$$

$$\mathcal{H}_{qrhk} := \frac{2}{\|\Delta \mathbf{C}\|^2} \Delta^{PF} b_{qr} \left( (\partial \Delta \mathcal{D}_{(1)}^{\text{int}})_{hk} - \xi_{t+\Delta t} \frac{\partial q_{t+\Delta t}}{\partial (\epsilon_{t+\Delta t}^{e,\text{trial}})_{hk}} \right) \quad (\text{A.26})$$

As it can be seen from Eq. (A.9), the derivative of the algorithmic Kirchhoff stress is multiplied by the deformation

512 gradient

$$\frac{\partial \tau_{qr}^{mp}}{\partial F_{mn}} F_{sn} = \mathcal{G}_{qrmn} F_{sn} + \left( \mathcal{F}_{qrab} \frac{\partial (\tau_{t+\Delta t})_{ab}}{\partial (\epsilon_{t+\Delta t}^{e,trial})_{hk}} + \mathcal{H}_{qrhk} \right) \frac{\partial (\epsilon_{t+\Delta t}^{e,trial})_{hk}}{\partial F_{mn}} F_{sn}. \quad (\text{A.27})$$

513 Therefore, some simplifications are possible

$$\begin{aligned} \mathcal{G}_{qrmn} F_{sn} = & \delta_{qm} \left( \frac{1}{2} (\tau_t^{PF})_{rs} + \frac{\Delta \mathcal{H}^{int}}{\|\Delta \mathbf{C}\|^2} \Delta^{PF} b_{rs} \right) + \delta_{rm} \left( \frac{1}{2} (\tau_t^{PF})_{qs} + \frac{\Delta \mathcal{H}^{int}}{\|\Delta \mathbf{C}\|^2} \Delta^{PF} b_{qs} \right) \\ & + \frac{\Delta \mathcal{H}^{int}}{\|\Delta \mathbf{C}\|^2} (b_{mp} b_{qs} + b_{qm} b_{rs}) - \frac{2}{\|\Delta \mathbf{C}\|^2} \Delta^{PF} b_{qr} \left( \bar{\tau}_{sm} - (\tau_{t+\Delta t})_{se} \bar{d}_{me} + 2 \frac{\Delta \mathcal{H}^{int}}{\|\Delta \mathbf{C}\|^2} \Delta^{PF} b_{sm} \right); \end{aligned} \quad (\text{A.28})$$

514

$$\mathcal{F}_{qrab} \left( \frac{\partial (\tau_{t+\Delta t})_{ab}}{\partial F_{mn}} \right) F_{sn} = \frac{1}{2} \mathcal{F}_{qrab} \mathcal{D}_{abhk}^{alg} \mathcal{L}_{hklu} \mathcal{B}_{lums}; \quad (\text{A.29})$$

515

$$\mathcal{H}_{qrhk} \frac{\partial (\epsilon_{t+\Delta t}^{e,trial})_{hk}}{\partial F_{mn}} F_{sn} = \frac{1}{2} \mathcal{H}_{qrhk} \mathcal{L}_{hklu} \mathcal{B}_{lums}, \quad (\text{A.30})$$

516 where the fourth-order tensors appearing in the above equations have been defined as

$$\mathcal{D}_{abhk}^{alg} := \frac{\partial (\tau_{t+\Delta t})_{ab}}{\partial (\epsilon_{t+\Delta t}^{e,trial})_{hk}}; \quad (\text{A.31})$$

$$\mathcal{L}_{hklu} := 2 \frac{\partial (\epsilon_{t+\Delta t}^{e,trial})_{hk}}{\partial (b_{t+\Delta t}^{e,trial})_{lu}} = \frac{\partial \log(b_{t+\Delta t}^{e,trial})_{hk}}{\partial (b_{t+\Delta t}^{e,trial})_{lu}}; \quad (\text{A.32})$$

$$\mathcal{B}_{lums} := \frac{\partial (b_{t+\Delta t}^{e,trial})_{lu}}{\partial F_{mn}} F_{sn} = (b_{t+\Delta t}^{e,trial})_{us} \delta_{lm} + (b_{t+\Delta t}^{e,trial})_{ls} \delta_{um}. \quad (\text{A.33})$$

517 The evaluation of the *consistent tangent modulus*  $\mathcal{D}_{abhk}^{alg}$  is not necessary, since it has been computed by the elasto-  
518 plastic subroutine.

519 The *spatial tangent modulus*  $\check{\alpha}_{prms}$ , defined in Eq. (A.9), can be therefore expressed as

$$\check{\alpha}_{prms} = \mathcal{P}_{prms} + \Theta_{prms} + \frac{1}{J} (\Delta F_{\Delta t - \theta}^{-1})_{pq} \left( \mathcal{G}_{qrmn} F_{sn} + \frac{1}{2} (\mathcal{F}_{qrab} \mathcal{D}_{abhk}^{alg} + \mathcal{H}_{qrhk}) \mathcal{L}_{hklu} \mathcal{B}_{lums} \right). \quad (\text{A.34})$$

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## A conservation law consistent updated Lagrangian material point method for dynamic analysis

Pretti et al. (2023)

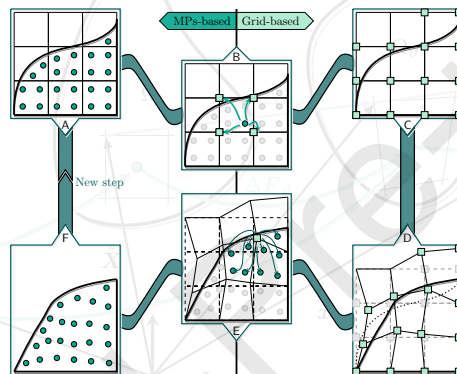
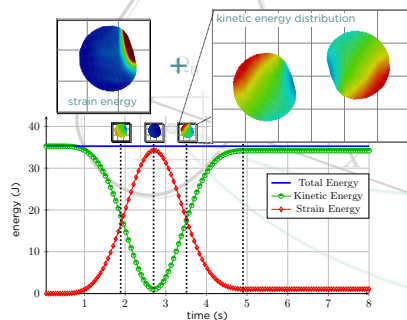


the conservation of energy is a core concept within physics and engineering

most numerical analysis codes artificially lose energy through numerical dissipation



in MPMs energy balance must be enforced at several steps as information is mapped between the material points and the background grid



Algorithm steps: (A) material points on background grid, (B) point-to-grid information mapping, (C) equilibrium equations formulated at nodes on the grid, (D) solve equilibrium equations for nodal motion, (E) grid-to-point motion & deformation mapping and (F) deformed body in equilibrium with external actions.

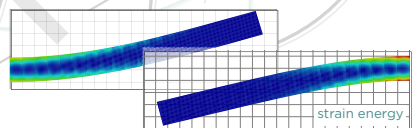


existing energy conserving MPMs are based on a Total Lagrangian (TL) description of motion

TL formulations require mesh deformations to be tracked, removing a key advantage of the MPM



a new energy conserving updated Lagrangian MPM is formulated that restores this key advantage



### Conclusion

The mass used in the point-to-grid and grid-to-point mappings is critical for energy conservation. A new energy conserving MPM for elasto-plastic analysis based on an updated Lagrangian description of motion is presented. Compatibility issues with total Lagrangian approaches and the MPM are avoided by this approach. This paper provides a platform for energy conservation studies for new methods under large deformations.

#### **Declaration of interests**

☐ The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

☒ The authors declare the following financial interests/personal relationships which may be considered as potential competing interests:

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