Monolithic coupling of implicit material point method with finite element method

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Abstract

A monolithic coupling between the material point method (MPM) and the finite element method (FEM) is presented. The MPM formulation described is implicit, and the exchange of information between particles and background grid is minimized. The reduced information transfer from the particles to the grid improves the stability of the method. Once the residual is assembled, the system matrix is obtained by means of automatic differentiation. In such a way, no explicit computation is required and the implementation is considerably simplified. When MPM is coupled with FEM, the MPM background grid is attached to the FEM body and the coupling is monolithic. With this strategy, no MPM particle can penetrate a FEM element, and the need for computationally expensive contact search algorithms used by existing coupling procedures is eliminated. The coupled system can be assembled with a single assembly procedure carried out element by element in a FEM fashion. Numerical results are reported to display the performances and advantages of the methods here discussed.

1 Introduction

The material point method (MPM) is a numerical method for problems that involve large deformations and/or history dependent materials. It has been originally introduced in [33, 35, 34] by Sulsky et al. as an extension to solid mechanics of the hydrodynamics FLIP method [7]. The MPM has been applied to simulate numerous problems involving, for instance: membranes [22, 42], granular materials [38, 5], sea ice modeling [36], explosions [18], free surface flows [40], snow modeling [30], viscoelastic fluids [29], phase-change [31], fluid-structure interaction [39, 16, 20], and dynamic crack propagation [19]. The MPM exploits the advantages of both the Eulerian and the Lagrangian approaches. The body is discretized with a set of particles (or material points) and is positioned on a background grid, where the momentum equation is solved. The background grid may be chosen to be a finite element grid, because interpolating functions are used to transfer information from the particles to the grid and back. In the classical MPM, particles information is transferred to the background grid, where the momentum equation is solved. The new information obtained from the solution of the momentum equation at the grid nodes is used to update the values of displacement, velocity and acceleration at the particles. Then, the background grid is reset to its initial position. With such a method, the drawbacks of using a purely Lagrangian approach are avoided, because entanglement of the background grid is prevented by resetting it to its initial state after every time step. Moreover, the numerical dissipation associated with an Eulerian approach is eliminated, due to the absence of the convection term.

Historically, the MPM has been conceived as an explicit method. Compared to the extensive amount of explicit MPM formulations available in the literature, only a few efforts have been made so far to set the analysis in an implicit framework [31, 37, 12, 27, 26, 6]. An implicit approach is desirable because it guarantees much larger time steps compared to what can be obtained with explicit methods, but more importantly the implicit formulation facilitates the monolithic coupling of the MPM with the FEM, which is the ultimate goal of the present work. As other existing implicit MPM formulations, here the assembly procedure for the problem on the background grid is carried out in a finite element fashion. The only difference between a standard FEM assembly is that, for elements of the background grid that enclose MPM particles, the quadrature points used for numerical integration are not the Gauss points as in standard FEM, but rather the particles themselves. The implicit MPM formulated here differs from existing implicit approaches [17, 37, 32, 27], because the exchange of information between particles and grid is minimized by avoiding unnecessary projections from the particles to the background grid nodes. In turn, as it is shown later, the inertial contribution is evaluated directly at the particles rather than at the grid nodes. This approach is consistent with an assembly procedure where the particles are used in

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The paper is structured as follows: in Section 2, the domain configurations later employed in the mathematical formulation are introduced. In Section 3, a detailed description of the implicit MPM formulation proposed is provided. The new features of our formulation and the complete numerical algorithm are presented and discussed. In Section 4, the monolithic coupling between MPM and FEM is addressed, and the characteristics of the coupled problem are laid out. In Section 5, an algorithm for the receding phase of the contact interaction is described. This algorithm is necessary in order to prevent sticky phenomena induced by our monolithic formulation for large values of the Young’s modulus. The paper is concluded with Section 6, where numerical results are reported to illustrate the performances of the proposed algorithms.

2 Domain Configurations

In this section, the domain configurations used in the mathematical formulation are discussed. A general description is given first, followed by the identification of what will be referred to as the MPM domain and the FEM domain. The problem of the reset of the MPM background at the beginning of every time step is addressed for both the uncoupled and the coupled case.

2.1 Three general domain configurations

Three different domain configurations are used in the mathematical formulation. The reason why the configurations are three is made explicit in the following sections. Let $T > 0$ and let $\Omega$ be a given open
and bounded domain such that, for all \( t \in [0, T] \), \( \Omega(t) \subset \mathbb{R}^d \). Then, the undeformed configuration of \( \Omega \) is indicated with the notation \( \hat{\Omega} \) and it represents the position of the domain in its original state at time \( t = 0 \). For the deformed configuration \( \Omega(t) \), no superscript is used, and the notation \( \Omega(t) \) just refers to the domain in its deformed configuration at time \( t > 0 \). This configuration is obtained from the undeformed configuration with a translation. Specifically, if \( \hat{x} \) represents any point of \( \hat{\Omega} \), then

\[
x(\hat{x}, t) = \hat{x} + u(\hat{x}, t), \quad \text{for } t > 0,
\]

where \( u(\hat{x}, t) \) is the displacement field. The third configuration to be introduced is the reference configuration, denoted by \( \bar{\Omega} \). We remark that, given \( n \geq 0 \), such a configuration does not change for any \( t \in (t^n, t^{n+1}] \). The reference configuration can also be obtained from the undeformed configuration with a translation, as follows

\[
\bar{x}(\hat{x}) = \hat{x} + u^{\text{reset}}(\hat{x}), \quad \text{for } t \in (t^n, t^{n+1}]
\]

where the field \( u^{\text{reset}} \) is referred to as the reset displacement field associated with the given time interval \( (t^n, t^{n+1}] \). The definition of such a field is given in the next section. Any point in the deformed configuration can be also obtained from the reference configuration as

\[
x(\hat{x}, t) = \bar{x} + \tilde{u}(\bar{x}, t), \quad \text{for } t \in (t^n, t^{n+1}]
\]

where the field \( \tilde{u} \) is the displacement field with respect to the reference configuration, which satisfies

\[
\tilde{u}(\bar{x}, t) = u(\hat{x}, t) - u^{\text{reset}}(\hat{x}), \quad \text{for } t \in (t^n, t^{n+1}].
\]

Schematics for the three domain configurations can be found in Figure 1.

The general considerations about domain configurations are applied to the MPM and FEM domains as explained next.

### 2.2 The MPM and the FEM domains

Let \( T > 0 \) and \([0, T] \subset \mathbb{R} \). For all \( t \in [0, T] \), let \( \Omega_{mpm}(t) \) and \( \Omega_b(t) \) be open and bounded subsets of \( \mathbb{R}^d \). Assume that \( \Omega_{mpm}(t) \subset \Omega_b(t) \) for all \( t \in [0, T] \). From now on, \( \Omega_{mpm}(t) \) represents the body discretized with the MPM particles. The set \( \Omega_b(t) \) is discretized with a regular finite element grid \( T_b \) used as a background grid for the MPM body. While \( \Omega_{mpm}(t) \) may be subject to roto-translation and large deformations due to the movement of the MPM body, \( \Omega_b(t) \) undergoes only limited deformations, because it follows the MPM body motion only in the time interval \((t^n, t^{n+1}]\). At the beginning of each time step, \( \Omega_b(t) \) is reset to its reference configuration \( \bar{\Omega}_b \), as it will be explained in the next section. Denoting by \( E_p \) the element of the background grid that hosts a given particle \( p \), we introduce

\[
\Omega_{ab}(t) \equiv \bigcup_{E \in T_{ab}} E = \bigcup_{p=1}^{N_p} E_{p}, \quad (4)
\]

where \( t \in (t^n, t^{n+1}] \), and \( T_{ab} \subset T_b \) is the active background grid, composed of all elements \( E \) of \( T_b \) that host at least one particle \( p \). Similarly, we define \( T_{ib} \equiv T_b \setminus T_{ab} \) to be the inactive background grid, composed

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Figure 1: Schematics for the domain configurations.
Figure 2: Schematics of triangulations and domains used in the MPM-FEM coupled problem. The nodes marked with a cross belong exclusively to the inactive background grid $\mathcal{T}_b$, while those marked with a box are the nodes at the interface between the MPM background grid $\mathcal{T}_b$ and the FEM grid $\mathcal{T}_{fem}$.

of all elements of $\mathcal{T}_b$ that do not enclose any particle. Note that the time dependence of $\Omega_{ab}(t)$ is due to the time dependence of $E_p$ (for given $p$) in the time interval $(t^n, t^{n+1}]$. Moreover, because the background grid is reset at the beginning of each time step, a particle $p$ may leave a particular element $E$ and move into one of its neighboring elements, so the elements of $\mathcal{T}_{ab}$ and $\mathcal{T}_b$ may also change at each time step. Schematics of the grids here described are shown in Figure 2. By definition, $\Omega_{ab}(t)$ has the property that $\Omega_{mpm}(t) \subseteq \Omega_{ab}(t) \subseteq \Omega_b(t)$. The set $\Omega_{ab}(t)$, associated with the MPM active background grid, is what we refer to as the MPM domain. Such a choice is motivated by the fact that the MPM momentum equation is solved only on the active background grid, and its elements consequently undergo deformations that modify their reference configuration.

Concerning the FEM, since the triangulation entirely covers the body to discretize, the open and bounded set $\Omega_{fem}(t) \subset \mathbb{R}^d$ is used to characterize both the body discretized with FEM and the FEM domain. The interfaces between the FEM domain and the background grid $\Omega_b(t)$ and between the FEM domain and the active background grid $\Omega_{ab}(t)$ that arise during the coupling procedure are indicated with the letters $\Gamma$ and $\Gamma_a$, respectively.

2.3 Definition of the reset displacement field

In the classical MPM method, where no coupling between MPM and FEM occurs, at the beginning of each time step interval $(t^n, t^{n+1}]$, the set $\Omega_b(t)$ is reset to its undeformed configuration, $\hat{\Omega}_b$, to avoid mesh entanglement. Namely, for any $t \in [t^n, t^{n+1}]$, if $I$ refers to any node of the grid, the grid displacement $u_I$ associated to the node $I$ is such that

$$\lim_{t \to (t^n)^+} u_I(t) = 0.$$  (5)

Moreover, in general

$$\lim_{t \to (t^n)^-} u_I(t) = u_I(t^n) \neq 0,$$  (6)

and as a result $u_I(t)$ is discontinuous in time. On the other hand, in the classical uncoupled FEM method, the grid follows the solid body deformation and its displacement is continuous in time

$$\lim_{t \to (t^n)^-} u_I(t) = u_I(t^n) = \lim_{t \to (t^n)^+} u_I(t).$$  (7)

With a monolithic coupling approach, there is a unique displacement field defined on the MPM background grid and on the finite element grid discretizing the FEM body. Hence, when the coupling between MPM and FEM is considered, the displacement at the grid points of $\hat{\Omega}_b$ that lie on the interface $\Gamma$ between $\Omega_b(t)$ and the FEM body cannot be reset to zero. This implies that at every instant of time, the deformed configuration of the MPM domain is composed of elements that are deformed, not only because of the motion of the MPM body, but also because of the FEM body motion.

The requirement of resetting the MPM background grid to its undeformed configuration at the beginning of every time step is what motivates the introduction of the reset displacement field to be used for the coupled problem. More specifically, when MPM is coupled with FEM, the background grid has to fulfill the following constraints: in the FEM domain and on the interface $\Gamma$, it has to follow the solid deformation; in the MPM domain, in order to enforce domain continuity, it has to follow the deformation of $\Gamma$, coming from the FEM domain. Moreover, to avoid mesh entanglement, it is desirable to reset the
background grid to a configuration similar to the undeformed configuration on all MPM nodes that are sufficiently far from $\Gamma$.

Because in the applications described in this paper the FEM solid body is subject to small deformations, the background grid constraints are satisfied with the following definition of the reset displacement field $u_I^{\text{reset}}$. Let $I$ be the set of grid points of $\mathcal{T} = \mathcal{T}_b \cup \mathcal{T}_{\text{fem}}$, where $\mathcal{T}_{\text{fem}}$ denotes the finite element grid used to discretize the FEM body. For all $t \in (t^n, t^{n+1}]$, the reset displacement field satisfies

$$
\begin{cases}
  u_I^{\text{reset}} = \lim_{t \rightarrow (t^n)^-} u_I(t), & \text{if } x_I \in \Omega_{\text{fem}}(t) \\
  \nabla \cdot (\nabla u_I^{\text{reset}} + (\nabla u_I^{\text{reset}})^T) = 0, & \text{if } x_I \in \Omega_b(t) \setminus \Gamma
\end{cases}
$$

(8)

where $x_I$ denotes the position of node $I \in I$. When MPM is coupled with FEM, Eq. (5) is replaced with

$$
\lim_{t \rightarrow (t^n)^+} u_I(t) = u_I^{\text{reset}}.
$$

(9)

By making this choice, continuity of the domain is preserved across $\Gamma$, and the grid motion. If the FEM body deformation is small, than the deformation of the background grid will also be small. To fulfill the classical MPM requirement in Eq. (5), a new MPM displacement field based on the reference configuration is defined as

$$
\tilde{u}_I(t) = u_I(t) - u_I^{\text{reset}}.
$$

(10)

By Eq. (9), this new field satisfies

$$
\lim_{t \rightarrow (t^n)^+} \tilde{u}_I(t) = 0,
$$

as in the classical uncoupled MPM method. The reference configuration is the configuration of the MPM domain associated with the field $\tilde{u}_I(t)$.

### 3 Implicit Material Point Algorithm

The mathematical formulation of the proposed implicit material point and the complete numerical algorithm are described in this section.

#### 3.1 Mathematical Formulation

For ease of notation, during the rest of this paper, the time dependence of $\Omega_{\text{mpm}}$, $\Omega_{\text{ab}}$, and of the fields involved in the formulation is not made explicit. The mass conservation is automatically satisfied by the material point method [41], therefore the governing equations for the MPM body consist of momentum conservation with appropriate boundary and initial conditions. For simplicity, we consider zero boundary conditions for displacement and normal stress

$$
\begin{align*}
\rho \ddot{u} - \nabla \cdot \sigma &= \rho b, & \text{in } \Omega_{\text{mpm}} \times [0, T], \\
\sigma \cdot n &= 0, & \text{on } \partial \Omega_{\text{mpm, trac}} \times [0, T], \\
u &= 0, & \text{on } \partial \Omega_{\text{mpm, disp}} \times [0, T], \\
u(x, 0) = u_0, & \dot{u}(x, 0) = \dot{u}_0 & \text{in } \Omega_{\text{mpm}}.
\end{align*}
$$

(11)

The case of Robin and mixed boundary conditions is not addressed at present. In Eq. (11), $u$ represents the displacement, $\sigma$ is the Cauchy stress tensor, $\rho$ is the MPM body density, $b$ is the body force per unit mass, $\dot{u}$ is the velocity, $\ddot{u}$ is the acceleration and $n$ is the unit outward normal of the boundary $\partial \Omega_{\text{mpm, trac}}$, that represents the traction boundary. Similarly, $\partial \Omega_{\text{mpm, disp}}$ represents the portion of the boundary where displacement boundary conditions are prescribed. Constitutive equations for the Cauchy stress need to be added to complete the above set of equations. We describe the MPM solid bodies as Neo-Hookean materials, with the Cauchy stress tensor given by [28]

$$
\sigma = \lambda \frac{\log(J)}{J} I + \mu \frac{1}{J} (B - I).
$$

(12)
In Eq. (12), \( \lambda \) is Lamé’s first parameter, \( I \) is the identity matrix, \( \mu \) is the shear modulus, \( B = FF^T \) is the left Cauchy-Green strain tensor, \( F \) is the deformation gradient and \( J = \det(F) \). Let \( \Delta U = \{ \delta u \in H^1(\Omega_{mpm}) \mid \delta u|_{\partial \Omega_{mpm}, \delta t = 0} = 0 \} \). The virtual displacements are chosen as test functions for the weak formulation. The weak formulation of the momentum balance reads

\[
\int_{\Omega_{mpm}} \rho \left( \ddot{u}_i \delta u_i + \sum_{j=1}^{d} \sigma_{ij}^s \frac{\partial \delta u_i}{\partial x_j} - b_i \delta u_i \right) dV = 0, \text{ for } i = 1, \ldots, d. \tag{13}
\]

where \( \sigma_{ij}^s = \sigma_{ij}/\rho(x, t) \) is the specific Cauchy stress. The interested reader can consult [1] for more details on how to derive the above weak formulation. The integrals involved in Eq. (13) can be transformed in sums if the MPM density \( \rho \) is approximated using the Dirac delta function \( \delta \) as

\[
\rho(x, t) \approx \sum_{p=1}^{N_p} m_p \delta(x - x_p(t)), \tag{14}
\]

where, \( x_p \) denotes the position of particle \( p \), and \( N_p \) represents the total number of particles used to discretize \( \Omega_{mpm} \). Note that the number of particles \( N_p \) is time independent, assuming that no particle is leaving \( \Omega_b \). Substituting Eq. (14) in Eq. (13) we obtain

\[
\sum_{p=1}^{N_p} m_p \left[ \ddot{u}_i(x_p) \delta u_i(x_p) + \sum_{j=1}^{d} \sigma_{ij}^s(x_p) \frac{\partial \delta u_i(x_p)}{\partial x_j} - b_i(x_p) \delta u_i(x_p) \right] = 0. \tag{15}
\]

In the above equation, \( \sigma_{ij}^s(x_p) = J(x_p) \sigma_{ij}(x_p)/\rho_0 \), where \( \rho_0 \) is the density of the MPM body in the initial, undeformed configuration.

**Remark 1.** Since the MPM body is discretized with particles, the values of the fields at the particles can be identified with the particle fields. For instance, \( \ddot{u}_i(x_p) = \ddot{u}_{i,p} \), where \( \ddot{u}_{i,p} \) represents the \( i \)-th component of the acceleration of particle \( p \).

Considering the above remark, Eq. (15) can be rewritten as

\[
\sum_{p=1}^{N_p} m_p \left[ \ddot{u}_{i,p} \delta u_i(x_p) + \sum_{j=1}^{d} \sigma_{ij}^s(x_p) \frac{\partial \delta u_i(x_p)}{\partial x_j} - b_{i,p} \delta u_i(x_p) \right] = 0. \tag{16}
\]

The weak formulation for the MPM equations in Eq. (16) is solved numerically employing the active background grid \( T_{ab} \). For any given particle \( p \), an interpolation from the nodes of the element \( E_p \in T_{ab} \) that encloses \( p \) is performed. This step is part of the assembly procedure of the background grid system and is discussed within the complete numerical algorithm.

### 3.2 Implicit Time Integration

In a time dependent framework, the position, displacement, velocity and acceleration of a given particle are functions of time. The Newmark-beta integrator is adopted for the numerical integration of \( \ddot{u}_{i,p} \) in Eq. (16). If \( \mathbf{u}_p^{n+1} \) denotes the particle displacement at time \( t^{n+1} \) and the same notation is also adopted for particle velocity and acceleration, the method gives

\[
\mathbf{u}_p^{n+1} = \mathbf{u}_p^n + (1 - \gamma) \Delta t \mathbf{u}_p^n + \gamma \Delta t \mathbf{u}_p^{n+1},
\]

\[
\mathbf{u}_p^{n+1} = \mathbf{u}_p^n + \Delta t \mathbf{u}_p^n + \frac{1}{2} \Delta t^2 (1 - 2\beta) \mathbf{a}_p^n + \Delta t^2 \beta \mathbf{a}_p^{n+1},
\]

for \( \gamma \in [0, 1] \), \( \beta \in [0, 0.5] \) and \( \Delta t = t^{n+1} - t^n \). It follows that,

\[
\mathbf{a}_p^{n+1} = \frac{1}{\beta \Delta t^2} \left( \mathbf{u}_p^{n+1} - \mathbf{u}_p^n \right) - \frac{1}{\beta \Delta t} \mathbf{a}_p^n - \frac{1 - 2\beta}{2\beta} \mathbf{a}_p^n.
\]

### 3.3 The numerical algorithm

The complete numerical algorithm for the implicit MPM scheme presented in this paper is described next. The algorithm is divided into a series of stages and it is set in a parallel framework where different processes handle their own share of the background grid and particles.
• Initialization of the MPM particles.

The first step consists of particle initialization. We assume that the total number of particles $N_p$, the volume $V_p$ associated with each particle, and the initial density $\rho_0$ of the undeformed MPM body are given. With this information, the mass of each particle is computed as $m_p = \rho_0 V_p$. The initial position $x_p$ of each particle $p$ is also known. The values of displacement $u_p$ and velocity $\dot{u}_p$ of the particles are initialized as in Eq. (11). The acceleration $\ddot{u}_p$ is set to zero, while the deformation gradient $F_p$ at the particle is initialized to a given initial value $F_p^0 \equiv F_p(0)$. Once a particle has been placed on the FEM background grid, the element $E_p$ on the background grid that hosts the particle is determined, using the point locating method described in [11]. As already mentioned above, such an element may be different over time, so for a given $p$, $E_p$ is actually a function of time.

For ease of notation, the time dependence is not made explicit. While for each $p$ the value of $E_p$ is known to all processes, the local coordinates $\xi_p$ of $p$ are computed only by the process that owns it, so the other processes do not possess this information. To obtain the local coordinates $\xi_p$ in the FEM reference configuration, an inverse mapping obtained with Newton’s method is employed. For more details on this procedure please see [11].

• Assembly and solution of the background grid system.

For this step, it is assumed that the particle instances at time $t^n$ are known and that those at time $t^{n+1}$ have to be determined. Let $\mathcal{T}_b = \{1, \ldots, N_b\}$ be the set of grid points of $\mathcal{T}_b$. Let $\mathcal{I}_{ab}$ be the set of grid points associated with $\mathcal{T}_{ab}$ and $\mathcal{I}_{db} = \mathcal{I}_b \setminus \mathcal{I}_{ab}$. The assembly procedure is carried out differently depending on whether a node of the background grid belongs to the active or inactive background grid. Both assembly procedures are described in detail in the next steps.

1. Assembly of the active background grid contributions.

A loop on the particles is executed to assemble the MPM contributions. Given a particle $p$ from the loop, the element $E_p$ on the active background grid $\mathcal{T}_{ab}$ that is currently hosting the particle is extracted. In a sense, this procedure is similar to a standard FEM procedure since the assembly is still performed in an element-by-element fashion. The differences are that now particles are used as quadrature points instead of Gauss points, and that the quadrature contributions on a given element are not computed sequentially, since particles that belong to the same element may not be all grouped together in the particle loop.

Remark 2. It is important to point out that, unlike other existing implicit MPM formulations [17, 37, 32, 27], our assembly procedure does not start with a mapping from the particles to the grid nodes. The Newmark scheme in Eq. (19) is used directly on the particle instances instead of the grid instances as existing strategies do. For this reason, no mapping from the particles to the background grid is necessary.

According to a FEM approach, the particle virtual displacement in Eq. (16) can be obtained through interpolation from the nodes of $E_p$. If $N_{\xi_p}$ denotes the number of nodes of element $E_p$, we have $\delta u_{i,p} = \sum_{I_{\xi_p}=1}^{N_{\xi_p}} \delta u_{i,I_{\xi_p}} \phi_{I_{\xi_p}}(x_p)$, where $\delta u_{i,I_{\xi_p}}$ represents the nodal value of the virtual displacement at node $I_{\xi_p}$ and $\phi_{I_{\xi_p}}$ is the finite element shape function associated with node $I_{\xi_p}$. Thanks to the arbitrariness of $\delta u_{i,I_{\xi_p}}$ and the fact that by definition $\delta u_{i,I_{\xi_p}} = 0$ on $E_p \cap \partial \Omega_{\text{mpm,disp}}$, the equation for the $I_{\xi_p}$-th entry of the local residual vector associated with MPM contributions is obtained from Eq. (16)

$$r_{\text{mpm},i,I_{\xi_p}} \equiv \sum_{p=1}^{N_p} m_p \left[ \ddot{u}_{i,p} \phi_{I_{\xi_p}}(x_p) + \left( \sum_{j=1}^{N_{\xi_p}} a_{i,j,p} \frac{\partial \phi_{I_{\xi_p}}}{\partial x_j}(x_p) \right) \right] - b_{i,p} \phi_{I_{\xi_p}}(x_p) = 0, \quad I_{\xi_p} = 1, \ldots, N_{\xi_p}. \tag{20}$$

In general, it may not be necessary to interpolate from the grid nodes to the particles to evaluate the body force at the particles. For instance, if the body force is a gravitational force, then no interpolation is necessary and its value at the particles can be computed directly. Therefore, the values of the body force remain evaluated at the particles, and interpolation may be performed if needed. The term $\ddot{u}_{i,p}$ in Eq. (16) is computed with the Newmark scheme in Eq. (19). Specifically, $\ddot{u}_{i,p}$ is given by

$$\ddot{u}_{i,p} = \frac{1}{\beta \Delta t^2} \dddot{u}_{i,p}(x_p) - \frac{1}{\beta \Delta t} \dot{u}_{i,p} - \frac{1 - 2\beta}{2\beta} \ddot{u}_{i,p}, \tag{21}$$
where \( \tilde{u}_{i,g}(x_p) \) denotes the reference background grid displacement value at \( x_p \), defined as

\[
\tilde{u}_{i,g}(x_p) \equiv \sum_{I_E=1}^{N_E} \tilde{u}_{i,I_E} \phi_{I_E}(x_p),
\]

where \( \tilde{u}_{i,I_E} \) is as in Eq. (10). The value of \( \sigma_{ij,p}^s \) in Eq. (20) refers to the specific Cauchy stress obtained with a partial interpolation from the grid nodes, as in [17]. Recalling the constitutive law in Eq. (12), \( \sigma_{ij,p}^s \) is given by

\[
\sigma_{ij,p}^s = \frac{\lambda}{J_p} \log(J_p) I + \mu \left( B_p - I \right),
\]

where \( J_p = \det(F_p) \), \( B_p = F_p (F_p)^T \) and

\[
F_p = \left( \nabla \tilde{u}_g(x_p) + I \right) F_p^0.
\]

In Eq. (24), \( \nabla \) represents the Del operator with respect to the reference configuration and \( \nabla \tilde{u}_g(x_p) \) is the background grid displacement gradient with respect to the reference configuration, evaluated at \( x_p \), defined as

\[
\nabla \tilde{u}_{i,j,g}(x_p) \equiv \sum_{I_E=1}^{N_E} \tilde{u}_{i,I_E} \frac{\partial \tilde{\phi}_{I_E}}{\partial x_j}(x_p).
\]

It is important to stress that if no coupling is considered, the undeformed configuration coincides with the reference configuration, since the reset displacement field is identically zero. This can be easily recalled considering Eq. (2).

The next step consists of determining the scaling factors to be used in the assembly of the soft stiffness matrix. Such factors depend on flags \( M_E \) assigned to each element of the active background grid \( T_{ab} \). The value of a flag depends on the element’s relative position with respect to the MPM particles. Let \( N_E \) be the total number of degrees of freedom associated with an element \( E \) on the active background grid. For instance, for bi-quadratic quadrilateral elements \( N_E = 9 \). See for instance Appendix A in [11] for a sketch of the Lagrangian bi-quadratic triangle and quadrilateral with associated degrees of freedom. For simplicity, we only consider the bi-quadratic case, but the following reasoning can be easily extended to linear and serendipity elements, as well as to higher dimensions. The value of the flag \( M_E \) is initialized to \( N_E \) for all elements in the active background grid. Let \( E \) be any of such elements. Then the value of \( M_E \) is modified according to the following criterion: for any node \( I_{E} \) of \( E \) that also belongs to an element of \( T_{ib} \), \( M_E \) is decreased by a unit. Hence, for instance, bi-quadratic quadrilateral elements that are surrounded by elements that do not enclose particles will have \( M_E = 1 \).

Next, a loop on all elements that are part of the active background grid is carried out in the standard finite element fashion, to compute the soft stiffness contribution of the local residual

\[
r_{soft,i,E} \equiv \mu C_E \int_{E} \left[ \nabla \tilde{u} + (\nabla \tilde{u})^T \right] : \nabla \tilde{\phi}_{I_E} dV, \quad \text{for} \quad I_{E} = 1, \ldots, N_E.
\]

The integral in Eq. (26) is approximated by means of a quadrature rule on the element \( E \), where Gauss points are used as quadrature points. The value of \( C_E \) is a measure of the magnitude of the soft stiffness contribution and it depends on the flags \( M_E \) previously determined. This is easily explained by the fact that the larger \( M_E \), the more elements filled with particles surround \( E \), and the smaller soft stiffness contribution is needed to stabilize the equations within \( E \). As a general rule, \( C_E \) is a non-increasing function of \( M_E \), and it is zero for any element fully surrounded by elements containing particles. The soft stiffness improves stability while decreasing accuracy. Accuracy decreases because a contribution that is not associated with the MPM problem is added to the system. As mentioned in the introduction, it is necessary to strike a balance between the need for accuracy and stability. A value of \( C_E = 0 \) is appropriate for elements that are fully surrounded by elements with particles but it may not be sufficient for those elements on the boundary of the MPM body. This is because they may not be filled enough with particles. It is recommended to keep \( C_E \) as small as possible, for instance in the interval \([10^{-2}, 10^{-8}]\). In the numerical simulations, we do not change the mass of the particles,
but we test our model for increasing values of the Young’s modulus $E$. As a consequence, the stiffness of the body increases, since $C_E$ is multiplied by $\mu$, which is proportional to $E$, while the gravitational force acting on the body remains the same. If the constant $C_E$ remains the same, the artificial stiffness proportional to $\mu C_E$ would increase. Hence, it is reasonable to decrease the value of $C_E$ at least proportionally to the increase of the Young’s modulus. A dimensionless analysis of the equation would confirm this straightforwardly. Examples of values for $C_E$ will be given in Section 4.

Note that Eq. (20) and Eq. (26) only involve nodes that belong to the active background grid $T_{ab}$, while the equation system at this stage is actually defined and solved for all the nodes of $T_b$. In such a way, there is no need to construct a new background grid at each instant of time, rather part of the background grid becomes active depending on the position of $\Omega_{mpm}$, as already explained above. For all nodes that belong to $T_{ab}$ (so exclusively to the inactive background grid), a fictitious equation is assembled using a lumped mass matrix, as it is shown next.

2. Assembly of the inactive background grid contributions.

Here, a loop on all the elements of the inactive background grid is carried out in a standard finite element fashion. Let $\mathcal{E}$ be any element in $T_{ab}$. Then, for any node $I_{\mathcal{E}} \in T_{ab}$, the local residual is computed as the product of a lumped mass matrix with the nodal displacement vector, as follows

$$r_{\text{mass},i,I_{\mathcal{E}}} \equiv \int_{\mathcal{E}} u_i,I_{\mathcal{E}} \bar{\phi}_{I_{\mathcal{E}}} dV \approx u_i,I_{\mathcal{E}} \left( \sum_{i_g=1}^{N_{E,g}} \bar{\omega}_i,i_g \bar{\phi}_{I_{\mathcal{E}}}(x_{i_g}) \right),$$

(27)

for $I_{\mathcal{E}} = 1, \ldots, N_{\mathcal{E}}, I_{\mathcal{E}} \in T_{ab}$. Recall that $T_{ab}$ contains only the nodes that belong exclusively to the inactive background grid, so nodes that are shared with elements that include at least one particle are excluded from the inactive background grid contribution. In Eq. (27), for $i_g = 1, \ldots, N_{E,g}$, $x_{i_g}$ is a Gauss point of the undeformed element $\hat{\mathcal{E}}$ associated with $\mathcal{E}$, $\bar{\omega}_i,i_g$ is the quadrature weight associated with $x_{i_g}$, and $u_i,I_{\mathcal{E}}$ is $i$-th component of the nodal displacement value at the local node $I_{\mathcal{E}}$, and $\bar{\phi}_{I_{\mathcal{E}}}$ is the shape function associated with node $I_{\mathcal{E}}$ of the undeformed element $\hat{\mathcal{E}}$.

3. Differentiation of the residual vector.

Let $r_{\text{mpm},E_p} = [r_{\text{mpm},1,1,1}, r_{\text{mpm},1,2,1}, \ldots, r_{\text{mpm},d,N_{E,p}}]$ denote the local residual vector associated with the MPM contributions from element $E_p$. The global MPM residual vector is denoted by

$$r_{\text{mpm}} = [r_{\text{mpm},1,1,1}, r_{\text{mpm},1,2,2}, \ldots, r_{\text{mpm},d,N_{E}}]$$

and is obtained in the standard finite element fashion, adding the entries of the local MPM residual vectors associated with the same global nodes. In the same way, the global soft residual vector $r_{\text{soft}}$ and the global mass residual vector $r_{\text{mass}}$ are constructed. It is important from an implementational point of view to ensure that the three global residual have matching dimensions and that they are all initialized to zero. Next, the global residual vector $r$ for the background grid system is defined as

$$r = r_{\text{mass}} + r_{\text{soft}} + r_{\text{mpm}},$$

(28)

Let $u^{k+1} = [u_{1,1}^{k+1}, u_{1,2}^{k+1}, \ldots, u_{d,N_{E}}^{k+1}]$ represent the vector of displacement values at the grid nodes at iteration $k + 1$, then $r(u^{k+1})$ is a nonlinear function of $u^{k+1}$ and to determine the values of the displacement at the grid nodes, it is necessary to solve the nonlinear equation

$$r(u^{k+1}) = 0.$$

(29)

Writing $u^{k+1} = u^k + \Delta u^{k+1}$ and expanding Eq. (29) in a Taylor series around $u^k$, the following equation is obtained

$$0 = r(u^{k+1}) = r(u^k) + \frac{\partial r(u^k)}{\partial u} \Delta u^{k+1} + O((\Delta u^{k+1})^2).$$

(30)

Neglecting the higher order terms, a linear system of equations is recovered

$$K(u^k) \Delta u^{k+1} = -r(u^k),$$

(31)
where $K(u^k) \equiv \frac{\partial r(u^k)}{\partial u}$ is the background grid stiffness matrix, $\Delta u^{k+1}$ is the solution increment vector and the forcing term $-r(u^k)$ is the negative residual vector associated with the solution at the previous iteration. In the numerical implementation, the matrix $K(u^k)$ is obtained using automatic differentiation provided by the Adept library \cite{21}. Hence, once the residual has been assembled, no explicit computation has to be carried out to obtain such a matrix.

After an appropriate reordering of the grid nodes, Eq. \((31)\) can be written as the following block system

$$
\begin{bmatrix}
K_{ab}(u_{ab}^k) & 0 \\
0 & M_{ib}
\end{bmatrix}
\begin{bmatrix}
\Delta u_{ab}^{k+1} \\
\Delta u_{ib}^{k+1}
\end{bmatrix}
= 
\begin{bmatrix}
-r_{ab}(u_{ab}^k) \\
-r_{ib}(u_{ib}^k)
\end{bmatrix},
$$

(32)

where

$$
K_{ab}(u_{ab}^k) = K_{soft}(u_{ab}^k) + K_{mpm}(u_{ab}^k),
$$

$$
r_{ab}(u_{ab}^k) = r_{soft}(u_{ab}^k) + r_{mpm}(u_{ab}^k),
$$

$$
K_{soft}(u_{ab}^k) \equiv \frac{\partial r_{soft}(u_{ab}^k)}{\partial u_{ab}}, \quad K_{mpm}(u_{ab}^k) \equiv \frac{\partial r_{mpm}(u_{ab}^k)}{\partial u_{ab}},
$$

$$
r_{ib}(u_{ib}^k) = r_{mass}(u_{ib}^k), \quad M_{ib} = \frac{\partial r_{mass}(u_{ib}^k)}{\partial u_{ib}}.
$$

4. Solution of the background grid system.

Let $\Delta u^{k+1}$ denote the solution of system \((32)\). With such an information, the displacement at the grid is advanced $u^{k+1} = u^k + \Delta u^{k+1}$. If the displacement falls below a prescribed tolerance, the algorithm moves to the next stage, otherwise further iterations are carried out.

- **Update of Particle Instances.**

In the last stage of the algorithm, the position, velocity, acceleration and deformation gradient of the particles are updated. As for the assembly procedure, this step begins with a loop on the particles. Then, for a given particle $p$ in the loop, the element $\mathcal{E}_p$ that hosts $p$ is again extracted. The deformation gradient is updated in the following way

$$
F_p^{n+1} = (\tilde{\nabla} \tilde{u}_p^{n+1}(x_p) + I) F_p^n,
$$

(34)

where

$$
\tilde{u}_p^{n+1}(x_p) \equiv \sum_{I_{\mathcal{E}_p}=1}^{N_{\mathcal{E}_p}} \tilde{u}_{I_{\mathcal{E}_p}}^{n+1} \tilde{\Phi}_{I_{\mathcal{E}_p}}(x_p).
$$

(35)

The particle displacement is obtained via interpolation from the displacement $\tilde{u}_I$ at the nodes of $\mathcal{E}_p$. Namely, $u_p^{n+1} \equiv \tilde{u}_p^{n+1}(x_p)$. With this information and the particle instances at the previous instant of time, velocity and acceleration are updated using the Newmark scheme in Eq. \((17)\) and Eq. \((19)\) respectively. Finally, the particle positions are updated as $x_p^{n+1} = x_p^n + u_p^{n+1}$.

4 Monolithic coupling between MPM and FEM

In this section, the solid-solid monolithic coupling between the proposed implicit material point method and the finite element method is described. The two solid bodies are treated as a single continuum, and a shared finite element grid is used for the FEM body and the MPM background grid. In this way, the MPM background grid follows the solid deformations and the interface between MPM and FEM bodies is automatically tracked. With this monolithic approach, there is no need for time consuming contact algorithms because the MPM particles do not penetrate the FEM body (conservation of mass). In addition, the continuity of the normal stress on the shared interface is automatically satisfied (conservation of momentum). The monolithic coupling used in this work is highly inspired by monolithic coupling strategies for fluid-structure interaction (FSI) problems \cite{9, 2, 10, 3, 4}. As a matter of fact, the MPM background grid is used in the same way as the finite element grid employed to discretize the fluid domain in FSI problems. In such problems, the displacement of the fluid grid at the interface is required to match the displacement of the solid grid. The same requirement is enforced here between the MPM background grid and the FEM solid grid. However, there is a major difference between the approach adopted in this
work and the one used to model FSI problems. Indeed, for any node of the background grid that does not belong to the FEM body, the displacement is reset to zero after every time step, as the MPM algorithm requires. On the other hand, such a reset does not occur for the fluid displacement in FSI problems. Another major difference is that of course no actual fluid equation is solved on the background grid in the present case, and the active background grid is only used for interpolation during the solution of the MPM equations.

The weak system of equations solved in the coupled case is the following

\[ \int_{\Omega_{ab}} \rho_{mpm} \left( \dot{u}_{mpm} \cdot \delta u_{mpm} + \sigma_{mpm}^s \cdot \nabla \delta u_{mpm} - b_{mpm} \cdot \delta u_{mpm} \right) dV \]
\[ - \int_{\Gamma_a} \rho_{mpm} (\sigma_{mpm}^s \cdot \delta u_{mpm}) \cdot n_{mpm} = 0, \quad \forall \delta u_{mpm} \in \Delta U_{mpm}, \]
\[ \int_{\Omega_{fem}} \rho_{fem} \ddot{u}_{fem} \cdot \delta u_{fem} + \sigma_{fem} \cdot \nabla \delta u_{fem} - \rho_{fem} b_{fem} \cdot \delta u_{fem} dV \]
\[ - \int_{\Gamma_a} (\sigma_{fem} \cdot \delta u_{fem}) \cdot n_{fem} = 0, \quad \forall \delta u_{fem} \in \Delta U_{fem}, \]

where \( \Delta U_{fem} \) represents the set of the test functions for the FEM weak formulation. Since two elastic bodies are simulated, the momentum equation is the same for both the MPM and the FEM body and the Cauchy stress is still given by Eq. (12) for both solids. Recall from Section 2.2 that \( \Gamma_a = \partial \Omega_a \cap \partial \Omega_{fem} \) denotes the interface between the MPM and the FEM domains. The continuity of mass and momentum between the equations in system (36) are satisfied. Namely,

\[ u_{mpm} = u_{fem} \]
\[ (\sigma \cdot n)|_{fem, \Gamma_a} + (\sigma \cdot n)|_{mpm, \Gamma_a} = 0, \tag{37} \]

where the second equation means that the FEM and the MPM values of \( (\sigma \cdot n) \) match on \( \Gamma_a \). Due to the monolithic approach, the equations for the MPM body and for the FEM body are solved at the same time with a unique assembly for the two. The assembly procedure is carried out exactly in the same way as in Section 3.3 for the nodes on the MPM background grid \( T_b \). If \( T_{fem} \) denotes the finite element grid used to discretize \( \Omega_{fem} \), let \( I_{fem} \) be the set of grid points of \( T_{fem} \). The inactive grid contributions are given only to the nodes in \( \Omega \setminus (T_{ab} \cup T_{fem}) \), so no coupling between inactive nodes and FEM nodes exists. For any node in \( I_{fem} \), the assembly procedure is carried out in a standard finite element fashion, using Gauss points as quadrature points. Recalling the constitutive law in Eq. (12), for a given Gauss point \( i_g \), we define \( \sigma_{ij,i_g} \) by

\[ \sigma_{ij} = \frac{\lambda_{fem} \log(J_{i_g})}{J_{i_g}} I + \frac{\mu_{fem}}{J_{i_g}} (B_{i_g} - I), \tag{38} \]

where \( J_{i_g} = \det(F_{i_g}) \), \( B_{i_g} = F_{i_g}(F_{i_g})^T \) and

\[ F_{i_g} = \left( \hat{\nabla} u_{i_g}(x_{i_g}) + I \right). \tag{39} \]

In Eq. (39), \( \hat{\nabla} u_{i_g}(x_{i_g}) \) represents the background grid displacement gradient with respect to the undeformed finite element configuration, evaluated at \( x_{i_g} \), given by

\[ \hat{\nabla} u_{ij,g}(x_{i_g}) = \sum_{I_E=1}^{N_E} u_{i,I_E} \frac{\partial \hat{\phi}_{I_E}}{\partial x_j}(x_{i_g}). \tag{40} \]

For any \( E \in T_{fem} \), the local residual is computed as

\[ r_{fem,i_g,I_E} = \sum_{i_g=1}^{N_{E}} \omega_{i_g} \left[ \ddot{u}_{i_g,I_E}(x_{i_g}) + \left( \sum_{j=1}^{d} \sigma_{ij,i_g} \frac{\partial \phi_{I_E}}{\partial x_j}(x_{i_g}) \right) \right] 
- \frac{\rho_{fem} b_{i_g,I_E}(x_{i_g})}{J_{i_g}} \phi_{I_E}(x_{i_g}) = 0, \quad \text{for } I_E = 1, \ldots, N_E. \tag{41} \]

Since particles are substituted by Gauss points in the FEM assembly, the Newmark scheme in Eq. (19) for the FEM body becomes

\[ \ddot{u}_{i_g}^{n+1} = \frac{1}{\beta \Delta t^2} \left( u_{i_g}^{n+1} - u_{i_g}^{n} \right) - \frac{1}{\beta \Delta t} \ddot{u}_{i_g}^{n} + \frac{1 - 2\beta}{2\beta} \ddot{u}_{i_g}^{n}, \tag{42} \]
where
\[ u_i^{n+1} = u_i^{n+1}(x_i) \equiv \sum_{I_k=1}^{N_{grid}} u_{I_k}^{n+1} \phi_{I_k}(x_i). \]  
(43)

The displacement, velocity and acceleration at the Gauss point at time \( t^n \) in Eq. (42) are computed in an analogous way as the displacement at the Gauss point at time \( t^{n+1} \) in Eq. (43). The coupled monolithic block system is again block diagonal and is given by
\[
\begin{bmatrix}
K_{ab}(u^k) & K_{ab,\text{fem}}(u^k) & 0 \\
K_{\text{fem},ab}(u^k) & K_{\text{fem}}(u^k) & 0 \\
0 & 0 & M_{ib}
\end{bmatrix}
\begin{bmatrix}
\Delta u_{ab}^{n+1} \\
\Delta u_{\text{fem}}^{n+1} \\
\Delta u_{ib}^{n+1}
\end{bmatrix}
= \begin{bmatrix}
-r_{ab}(u^k) \\
-r_{\text{fem}}(u^k) \\
-r_{ib}(u^k)
\end{bmatrix},
\]
(44)

where
\[
K_{ab}(u^k) = K_{\text{soft}}(u^k) + K_{\text{mpm}}(u^k),
\]
\[
r_{ab}(u^k) = r_{\text{soft}}(u^k) + r_{\text{mpm}}(u^k),
\]
\[
K_{\text{soft}}(u^k) = \frac{\partial r_{\text{soft}}(u^k)}{\partial u_{ab}},
\]
\[
K_{\text{mpm}}(u^k) = \frac{\partial r_{\text{mpm}}(u^k)}{\partial u_{ab}},
\]
\[
K_{ab,\text{fem}}(u^k) = \frac{\partial r_{\text{ab}}(u^k)}{\partial u_{\text{fem}}},
\]
\[
K_{\text{fem,ab}}(u^k) = \frac{\partial r_{\text{fem}}(u^k)}{\partial u_{ab}},
\]
\[
r_{ib}(u^k) = r_{\text{mass}}(u^k),
\]
\[
M_{ib} = \frac{\partial r_{\text{mass}}(u^k)}{\partial u_{ib}}.
\]

The (1,2) and (2,1) blocks represent the coupling between the active background grid and the FEM body nodes. After the solution of the monolithic system, the nodal values of velocity and acceleration at the grid nodes in \( I_{\text{fem}} \) are updated using the Newmark scheme
\[
\ddot{u}_i^{n+1} = \frac{1}{\beta \Delta t^2} (u_i^{n+1} - u_i^n) - \frac{1}{\beta \Delta t} \dot{u}_i^n - \frac{1 - 2 \beta}{2 \beta} \ddot{u}_i^n,
\]
\[
\dot{u}_i^{n+1} = \dot{u}_i^n + \Delta t \left( (1 - \gamma) \ddot{u}_i^n + \gamma \ddot{u}_i^{n+1} \right).
\]
(46)

5 Receding Contact Force Correction

The MPM domain may be subject to roto-translation and large deformations, and it is possible for its boundary to come into contact with the domain boundary where a Dirichlet boundary condition is imposed or with the FEM solid boundary. These situations require the contact force modeling to be carefully described. The contact force between two surfaces acts only when they touch, and a mutual pressure is applied. During the receding phase, when the bodies detach, the contact force must be zero. Moreover, penetration between the touching domains should never occur. The proposed monolithic formulation never allows for penetration, and the force balance at the interface is automatically satisfied in the touching phase of the contact. However, in the receding phase, the contact suffers of small to moderate sticky effects, that grow with increasing values of the Young’s modulus of the MPM body.

To avoid the artificial stickiness in the receding phase, a simple correction to the contact description is embedded in the implicit monolithic formulation. The correction requires a small modification in the MPM assembly for those elements of the active background grid for which a face is shared with an element of the FEM body, or Dirichlet boundary conditions are imposed on it. The nodal displacement values of such elements receive an additional contribution for each enclosed particle that moves away from the face. The idea is to reduce the reaction force exerted by the face in the evaluation of \( F_p \) in Eq. (44).

In particular, a reduction of the contribution of \( \tilde{V} \tilde{u}_p(x_p) \) to the deformation gradient \( F_p \) is obtained. The algorithm has been implemented here only for bi-quadratic Lagrangian quadrilateral elements but it readily extends to other shapes and families of finite elements. Let \( p \) be a particle and let \( E_p \) be the element that encloses it, depicted in Figure 5. For simplicity, we consider the case where Dirichlet zero boundary conditions have been imposed on the lower face of \( E_p \). Hence, the lower face will remain undeformed in the time interval \( [t^n, t^{n+1}] \). This implies that \( \tilde{u}_1 = \tilde{u}_2 = \tilde{u}_5 = 0 \), whereas the other nodes are free to move, see the dashed gray contour in Figure 3. If the particle moves away from the Dirichlet
boundary, the values of $\tilde{u}_{I_{E}p}$, with $I_{E}p = 1, \ldots, N_{E}p = 9$, are modified as follows

$$\tilde{u}_{1}^{*} = (1 - C_{c})\tilde{u}_{1} + C_{c}\left(\frac{4}{3}\tilde{u}_{4} - \frac{1}{3}\tilde{u}_{8}\right),$$

$$\tilde{u}_{2}^{*} = (1 - C_{c})\tilde{u}_{2} + C_{c}\left(\frac{4}{3}\tilde{u}_{3} - \frac{1}{3}\tilde{u}_{6}\right),$$

$$\tilde{u}_{5}^{*} = (1 - C_{c})\tilde{u}_{5} + C_{c}\left(\frac{4}{3}\tilde{u}_{7} - \frac{1}{3}\tilde{u}_{9}\right),$$

$$\tilde{u}_{I_{E}p}^{*} = \tilde{u}_{I_{E}p} \text{ for } I_{E}p = 3, 4, 6, 7, 8, 9,$$

with $C_{c} \in [0, 1]$. Note that the terms multiplied by $C_{c}$ in the above equations represent the correction terms. The new deformation field allows the nodes on the lower face to move, see the dashed red line in Figure 3. For $C_{c} = 0$, the Dirichlet boundary condition is restored. For $C_{c} = 1$, the new displacement field is such that $\nabla \tilde{u}_{I_{E}p}^{*}(x_{1}) = \nabla \tilde{u}_{I_{E}p}^{*}(x_{2}) = \nabla \tilde{u}_{I_{E}p}^{*}(x_{5}) = 0$, and consequently for each particle $p$ located on the lower face it would be

$$\mathbf{F}_{p} = \left(\nabla \tilde{u}_{I_{E}p}^{*}(x_{p}) + \mathbf{I}\right)\mathbf{F}_{p}^{n} = \mathbf{F}_{p}^{n},$$

with no new contribution to the stress tensor. For $C_{c} \in (0, 1)$, the resulting boundary condition can be considered of mixed type. The equations in (47) can be used also for the case of non zero Dirichlet boundary condition or contact of the MPM body with the FEM body.

The value of the constant $C_{c}$ has been investigated numerically. It is shown in Section 6 that if an MPM body rolls on a boundary (or on a FEM body), one can choose $C_{c} = 0.5$ regardless of the material type, the grid resolution and the coefficients $C_{E}$ for the soft stiffness matrix. For the case of a bouncing MPM object on a FEM plate, the numerical results show sensitivity to $C_{c}$, and a different value has to be chosen any time one of the parameters changes. However, it will be shown that the range of values of $C_{c}$ remains small.

6 Numerical Results

Numerical results are presented in this section to showcase the performances of the algorithms here described. First, the implicit MPM scheme is tested, followed by the monolithic coupling between MPM and FEM. When possible, the numerical results are compared to analytic solutions to show the great accuracy of the methods presented. For simplicity, only 2-dimensional numerical tests are performed, even if the methods developed in this work readily apply to 3-dimensional problems as well.

6.1 Initialization of the MPM Bodies

In the following numerical examples, two different types of MPM bodies are considered, a disk and a beam. Both bodies have a uniform particle distribution in their core and a progressively refined distribution moving from an a priori chosen interior surface towards the boundary. Recall that the particle mass is defined as $m_{p} = \rho_{0}V_{p}$, where $\rho_{0}$ is the initial density of the MPM body and $V_{p}$ is the particle volume. This volume has a value that depends on the location of the particle within the particle distribution used to discretized the body. Two different initialization procedures are carried out depending on the specific body.
6.1.1 Initialization of the disk

The input parameters for the disk are: the coordinates of the center of the disk \((x_c, y_c)\), the radius of the disk \(R\), the radius of the interior disk in which the uniform distribution is built \(R_b\), and \(N_b\), which is the number of particles located within the disk of radius \(R_b\). The number of boundary layers \(N_b\) between the circles can be obtained after \(R, R_b, \) and \(N_b\) have been chosen. For each particle, the output parameters are its initial coordinates and its volume \(V_p\).

6.1.2 Initialization of the beam

The input parameters for the beam are: the coordinates of the center point of the left boundary \((x_0, y_0)\), the height \(H\) and length \(L\) of the beam, the height \(H_0\) of the interior beam in which a uniform distribution is built, and the number \(N_{bH}\) of particle rows in the interior beam. The number of boundary layers \(N_b\) between the beams can be obtained once \(H, H_0\) and \(N_{bH}\) are chosen. For each particle, the output parameters are again its initial coordinates and its volume \(V_p\).

The pseudocode for the initialization of the two MPM bodies is given in Appendix A. We remark that the performances of the method do not depend on the specific particle distribution adopted in this work and other distributions may be possible.

6.2 Tests for the implicit MPM

We begin by considering a 2-dimensional example of a disk rolling on an inclined plane. The case of a rolling disk (or ball in 3D) is a common test for the MPM, and it has been used in several other works, we report for instance [5, 13, 24]. The plane has an inclination of \(\theta = \pi/4\), and Young’s modulus \(E\). Two values of \(E\) are chosen for the simulations, \(E_1 = 4.2 \times 10^8 \text{ Pa}\) and \(E_2 = 4.2 \times 10^8 \text{ Pa}\). The coarse mesh is composed of 4 horizontal layers, each with 20 bi-quadratic quadrilateral elements, so each of them has unitary length in the \(x\)-direction. Because the mesh is progressively refined moving towards the plane, each layer has a different cell size in the \(y\)-direction. These lengths are 1.72 \(m\), 1.34 \(m\), 1.09 \(m\), and 0.85 \(m\). Finer grids are obtained with midpoint refinement. Hence, after every refinement, the number of elements increases by a factor of four. Let \(J\) denote the number of refinements carried out for a given simulation. For instance, if \(J = 3\), the coarse background grid is refined 3 times. If \(J = 0\), it means that the coarse grid is not refined. The values of \(J = 1, 2, 3, 4\) are chosen for the tests. The initial distance \(d_0(J)\) of the center of the disk from the plane depends on the refinement of the grid, and it is designed to keep a small gap between the disk and the plane. For given \(J\) and \(E\), the gap is a fraction of the height of the element of the background grid where the contact occurs. We choose \(d_0(J) = R + 0.2/2^{J-1}\) for \(E_1\), and \(d_0(J) = R + 0.3/2^{J-1}\) for \(E_2\). The reference frame is translated and centered at the center of the disk as in Figure 4. The analytic expression of the \(x\)-coordinate of the center of mass assuming an undeformable disk is given by

\[
x(t) = x_0 + \frac{1}{3} g t^2 \sin(\theta),
\]

where \(x_0\) is assumed to be zero. Concerning the other simulation parameters, the density of the disk is \(1000 \text{ kg/m}^3\), the Poisson’s coefficient is \(\nu = 0.4\), and the step size is \(\Delta t = 0.01 \text{ s}\). For Newmark’s integrator, \(\beta = 0.3\) and \(\gamma = 0.5\) are selected. Rolling without slip is considered and \(C_e = 0.5\). The input parameters for the generation of the disk are \((x_c, y_c) = (0, 0), R_b = 1.4 \text{ m}, R = 1.6 \text{ m}, N_b = 300,\) and \(N_b = 22\), for a total of 48739 particles. The pseudocode for the initialization of the MPM disk can be found in Appendix A. In Figure 5 the particle distribution (including the particle boundary layers) and some details about the graded mesh for the background grid are visible. In Figure 5 the values of
The different shades of gray for the elements of the background grid identify different values of $M_E$, which is referred to as Mat in the legend. One refinement ($J = 1$) has been considered for the background grid.

| $E$     | $C_E$   | $J = 1$  | $J = 2$  | $J = 3$  | $J = 4$  |
|---------|---------|----------|----------|----------|----------|
| $4.2 \cdot 10^6$ | Eq. (50) | 5.545e-02 | 3.921e-02 | 2.571e-02 | 2.253e-02 |
| $4.2 \cdot 10^8$ | Eq. (51) | 4.520e-02 | 3.502e-02 | 2.423e-02 | 1.720e-02 |

Table 1: averaged relative error associated with the results in Figure 6

The flags $M_E$ are also reported for the elements of the background grid. Recall that since bi-quadratic elements are considered, the maximum possible value of $M_E$ is 9, which is attained for interior elements. The lightest gray refers to the elements of the inactive background grid. The following values were chosen for the soft stiffness scaling factor $C_E$ in Eq. (26)

For $E_1$: $C_E = \begin{cases} 
10^{-3} & \text{if } M_E < 5, \\
10^{-7} & \text{if } 5 \leq M_E < 9, \\
0 & \text{if } M_E = 9,
\end{cases}$

(50)

For $E_2$: $C_E = \begin{cases} 
10^{-5} & \text{if } M_E < 5, \\
10^{-9} & \text{if } 5 \leq M_E < 9, \\
0 & \text{if } M_E = 9.
\end{cases}$

(51)

The horizontal position of the center of mass obtained numerically solving our implicit MPM scheme is compared to the analytic expression in Eq. (49) for different values of $J$, and $E$. Results for $E_1$ are visible in Figure 6(I), for different mesh sizes. The curves obtained with the proposed implicit MPM method are in agreement with the analytic equation of the center of mass in Eq. (49). It is also shown that a progressive refinement of the mesh provides increasingly accurate results, since the curve associated with $J = 4$ is the one that best overlaps with the analytic expression. Results for $E_2$ are reported in Figure 6(II). Once again, the curves are in agreement with the analytic expression and larger values of $J$ give better accuracy.

Average relative errors are also shown, to provide a quantitative measure of the error. If $x(t)$ represents the position of the center of mass defined in Eq. (49), let $\bar{x}(t)$ be the position computed with the proposed method. Then the averaged relative error is defined as

$$\frac{1}{N_t} \sum_{i=1}^{N_t} \left| \frac{x(t_i) - \bar{x}(t_i)}{x(t_i)} \right|,$$

(52)

where $N_t = 250$ is the total number of time steps considered. Results for the above error are reported in Table 1 corresponding to the curves in Figure 6.

The section continues with simulations of a cantilever beam with length $L = 0.625$ m and height $H = 0.25$ m, visible in Figure 7. The parameters to build the MPM beam are $(x_0, y_0) = (0, 0)$, $L = 0.625$ m, $H = 0.25$ m, $H_0 = 0.15$ m, $N_H = 20$, and $N_v = 21$, for a total of 23041 particles. The pseudocode for the MPM beam initialization is given in Appendix A. The domain is a unit box, whose center of the left boundary is placed at the origin, and the coarse mesh is composed of 4 bi-quadratic quadrilateral elements. The background grid obtained when $J = 2$ is visible in Figure 7. The beam has density $\rho = 10,000$ kg/m$^3$, Poisson’s coefficient $\nu = 0.4$, and Young’s modulus $E = 1.74 \cdot 10^6$ Pa. The step size
is $\Delta t = 0.008$ s and, as before, $\beta = 0.3$ and $\gamma = 0.5$ are chosen for Newmark’s integrator. The values of $C_E$ are

For $E_2$: $C_E = \begin{cases} 10^{-6} & \text{if } M_E < 5, \\ 10^{-10} & \text{if } 5 \leq M_E < 9, \\ 0 & \text{if } M_E = 9. \end{cases}$ (53)

The simulation is carried out in the following way: the beam is initially subject to its self weight, so only the gravitational force is applied to it. Then, when it reaches its largest deformation, is assumed that the gravitational force is removed and the oscillations of the tip of the beam are monitored. If no significant damping in the oscillations can be observed as time increases, it means that the method is accurate. Graphs for such oscillations are reported in Figure 8 for values of $J = 2$, $J = 3$ and $J = 4$. From Figure

![Figure 7: Cantilever beam simulation with $J = 2$. The MPM particles are omitted on the right figure to highlight the deformations and the values of $M_E$ for the background grid elements.](image-url)

it can be seen that, as time increases, the oscillations became slightly off-phase as the mesh becomes finer. Although, the damping of the oscillations is very small, for all mesh sizes considered, despite the long duration of the simulation which is 8 seconds.
6.3 Tests for the MPM-FEM coupling

In this section, numerical results for the MPM-FEM coupling are presented. We begin by considering a disk rolling on an inclined plate, as in [24, 13]. The disk is modeled with MPM while the plate is discretized with FEM. The dimensions of the plate are $20 \times 1.6 \text{ m}$ while the radius of the disk is $R = 1.6 \text{ m}$. Rolling without slip is considered and the inclination of the plate is $\theta = \pi/4$. The MPM background grid is the same as the one used for the rolling ball in the uncoupled case, whereas for the FEM plate two horizontal layers of 20 elements each are considered, with $x$ length $1 \text{ m}$ and $y$ length $0.85 \text{ m}$. Recall that the use of a background grid for the MPM attached to the FEM body is one of the major contributions of the present work. The coupling coefficient $C_c$ is equal to 0.5. The coarse grid is refined by means of midpoint refinement, with $J$ indicating the number of refinements performed. The density and the Poisson’s coefficient of both the disk and the plate are set to $1000 \text{ kg/m}^3$ and $\nu = 0.4$, respectively. For what concerns the time integration, $\Delta t = 0.01 \text{ s}$, and the parameters for Newmark’s integrator are $\beta = 0.3$ and $\gamma = 0.5$. The Young’s moduli of the MPM and the FEM bodies are respectively $E_{\text{mpm}} = 4.2 \cdot 10^6 \text{ Pa}$ and $E_{\text{fem}} = 8.4 \cdot 10^6 \text{ Pa}$, with $\alpha = 6, 7, 8$. The initial vertical distance $d_0$ of the center of the disk from the plane is $d_0 = R + 0.15/2^{J-1}$ for $\alpha = 6$, $d_0 = R + 0.2/2^{J-1}$ for $\alpha = 7$, and $d_0 = R + 0.25/2^{J-1}$ for $\alpha = 8$. Again this is done so that there exists an initial small gap between the disk and the plane, and it is designed so that the gap dimension is a fraction of the height of the background grid element where the contact occurs. The reference frame is then translated and centered at the center of mass of the disk, hence the analytic expression of the $x$-coordinate of the center of mass is given in Eq. (49). The parameters for the initialization of the MPM disk are now $(x_c, y_c) = (0, 0)$, $R = 0.16 \text{ m}$, $R_0 = 0.14 \text{ m}$, $N_{\theta_0} = 600$ and $N_b = 24$, for a total of 57084 particles. The coefficient $C_E$ for the present tests has been chosen as follows:

For $\alpha = 6$: $C_E = \begin{cases} 10^{-2} & \text{if } M_E < 5, \\ 10^{-6} & \text{if } 5 \leq M_E < 9, \\ 0 & \text{if } M_E = 9, \end{cases}$ (54)

For $\alpha = 7$: $C_E = \begin{cases} 10^{-3} & \text{if } M_E < 5, \\ 10^{-7} & \text{if } 5 \leq M_E < 9, \\ 0 & \text{if } M_E = 9. \end{cases}$ (55)

For $\alpha = 8$: $C_E = \begin{cases} 10^{-4} & \text{if } M_E < 5, \\ 10^{-8} & \text{if } 5 \leq M_E < 9, \\ 0 & \text{if } M_E = 9. \end{cases}$ (56)

In Figure 8, results are displayed for $\alpha = 6, 7, 8$. We observe that also in the coupled case there is agreement between the numerical results and the analytic position of the center of mass. Once again, increasing the value of $J$ provides better accuracy with respect to the analytic curve. Moreover, to stiffer materials it corresponds a smaller error. This is also expected since the analytic solution is obtained under the assumption of an undeformable body. The averaged relative errors reported in Table 2 confirm the accuracy and validity of the proposed coupling method. This section is concluded with simulations.
of a disk falling from above and bouncing on a horizontal plate. As before, the disk is modeled with MPM and the plate is discretized with FEM. The coarse MPM background grid has dimensions $1.28 \times 1.84 \text{m}$ and it is made of 80 elements of $x$ length 0.16 m and $y$ length 0.184 m. The FEM plate has dimensions $1.28 \times 0.64 \text{m}$ and is discretized with 2 horizontal layers of 8 cells each, of $x$ length 0.16 m and $y$ length 0.08 m. The disk has radius $R = 0.16 \text{m}$ and is placed initially at the center-top of the background grid such that its distance from the upper surface of the plate is 1.68 m. Schematics of the coarse background grid and discretizations are visible in Figure 10 while a picture of the impact between the disk and the plate can be found in Figure 11. The parameters for the initialization of the MPM disk are now $(x_c, y_c) = (0, 0)$, $R = 0.16 \text{m}$, $R_0 = 0.14 \text{m}$, $N_{\theta_0} = 300$ and $N_{b} = 22$, for a total of 48739 particles. For what concerns the physical parameters, both the disk and the plate have density
Figure 10: Disk falling on a horizontal plate. The disk (white) is modeled with MPM, and the plate (black) with FEM. The coarse background grid is in gray color.

Figure 11: Deformation of the disk and plate as the disk impacts on the plate.

\[ \rho_{\text{mpm}} = \rho_{\text{fem}} = 1000 \text{ kg/m}^3 \] and Poisson’s coefficient \( \nu = 0.4 \). The Young’s moduli for the MPM and FEM body are, respectively, \( E_{\text{mpm}} = 5.91 \cdot 10^6 \text{ Pa} \) and \( E_{\text{fem}} = 4.2 \cdot 10^7 \text{ Pa} \). The aim of these tests is to further demonstrate the accuracy of the proposed methods and to highlight how it improves as the values of the coefficient \( C_E \) is decreased, considering fixed values of \( E \). This behavior is explained by the fact that for fixed Young’s modulus, smaller values of \( C_E \) decrease the soft stiffness contribution and therefore decrease the error added to the method. The values of \( C_E \) for this example are as follows:

\[
C_{E,1} = \begin{cases} 
10^{-2} & \text{if } M_E < 5, \\
10^{-6} & \text{if } 5 \leq M_E < 9, \\
0 & \text{if } M_E = 9,
\end{cases} \tag{57}
\]

\[
C_{E,2} = \begin{cases} 
10^{-5} & \text{if } M_E < 5, \\
10^{-9} & \text{if } 5 \leq M_E < 9, \\
0 & \text{if } M_E = 9.
\end{cases} \tag{58}
\]

The value of the coupling coefficient \( C_c \) depends on the refinement level and on \( C_E \) in this case. Its values are reported in Table 3. To speed up the simulation, the time stepping is adaptive, meaning that \( \Delta t \) is large when the disk is far from the plate and it is suddenly decreased after the disk reaches a given distance from the plate. The value of \( \Delta t \) when the disk is near the plate is reported in Table 3. The parameters for Newmark’s integrator are once again \( \beta = 0.3 \) and \( \gamma = 0.5 \).

The results for \( C_{E,1} \) are displayed in Figure 12 I), where the vertical position of the center of mass is tracked as time increases. It is assumed that the reference frame is positioned on the initial position of the center of mass and that the plate is not subject to the gravitational force, to avoid oscillations not caused by the impact. As the refinement of the background grid increases, a slight offset between the curves is observed, the magnitude of which increases with time. An analogous situation was observed in Figure 8 for the case of an oscillating cantilever beam. A different situation is displayed in Figure 12 II), for \( C_{E,2} \). Compared to Figure 12 I), it can be seen that the offset is considerably reduced and now all the curves
Table 3: Contact constant $C_e$ and step size near the plate $\Delta t_{plate}$ for the bouncing disk case.

| $J$   | $C_{E,1}$ | $C_{E,2}$ |
|-------|-----------|-----------|
| 2     | 0.06      | 0         |
| 3     | 0.1       | 0.2       |
| 4     | 0.2       | 0.2       |

| $J$   | $\Delta t_{plate}$ (sec) |
|-------|--------------------------|
| 2     | 0.0005                   |
| 3     | 0.00025                  |
| 4     | 0.000125                 |

Figure 12: Vertical position of the center of mass of a disk bouncing on a plate. I) $C_e = C_{E,1}$ defined in Eq. (57). II) $C_e = C_{E,2}$ defined in Eq. (58).

are in better agreement, especially those for $J = 3$ and $J = 4$. In both cases shown, no damping of the oscillations is observed, once again confirming the reliability and accuracy of our monolithic coupling. In conclusion, the results presented here show that, for fixed values of the Young’s modulus, it is important for the accuracy to choose the least possible values of $C_e$ that guarantees the convergence of the method.

7 Conclusion

A new coupling procedure between the material point method and the finite element method has been presented. The material point method has been formulated implicitly, and unnecessary exchanges of information between the particles and the background grid have been avoided, resulting in an improved accuracy compared to the case where this transfer of information is performed. The coupling with the finite element method has been carried out in a monolithic fashion, eliminating the need for time consuming contact search algorithms used by existing strategies to determine the relative position of the bodies. While numerical results have shown accuracy and reliability of the newly developed monolithic coupling procedure, further work has to be done to explore its capabilities. For instance, different types of couplings other than solid-solid will be investigated, as well as techniques to use our monolithic approach
for the coupling of the MPM with a fluid-structure interaction framework.

Appendix A

Initialization of the MPM disk pseudocode:

Input Parameters: \( x_c, y_c, R, R_0, N_{\theta_0}, N_b \) (with \( N_b \geq \frac{R - R_0}{R_0} \) ceil \( \frac{N_{\theta_0}}{2\pi} \))

\[ N_r = \text{ceil}\left(\frac{N_{\theta_0}}{2\pi}\right), \quad \Delta R = \frac{R_0}{N_r} \]

#Uniform Distribution

\[ p = 1, \quad x_p = x_c, \quad y_p = y_c \]

for \( i = 0, ..., N_r - 1 \)

\[ r_i = R_0 - i \Delta R, \quad N_{\theta_i} = \text{ceil}\left(\frac{N_{\theta_0} r_i}{R_0}\right), \quad \Delta \theta_i = \frac{2\pi}{N_{\theta_i}} \]

for \( j = 0, ..., N_{\theta_i} - 1 \)

\[ p = p + 1, \quad x_p = x_c + r_i \cos(j \Delta \theta_i), \quad y_p = y_c + r_i \sin(j \Delta \theta_i) \]

end for

end for

for \( i = 1, ..., p \)

\[ m_p = \rho_{mpm} \frac{\pi R_0^2}{p} \]

end for

#Boundary Layers

Find \( a \) such that \( \sum_{k=1}^{N_b} \Delta R a^k = R - R_0 \)

for \( i = 1, ..., N_b \)

\[ r_i = R_0 + \sum_{k=1}^{i} \Delta R a^k, \quad N_{\theta_i} = \text{ceil}\left(\frac{N_{\theta_0}}{a^i}\right), \quad \Delta \theta_i = \frac{2\pi}{N_{\theta_i}} \]

for \( j = 0, ..., N_{\theta_i} - 1 \)

\[ p = p + 1, \quad x_p = x_c + r_i \cos(j \Delta \theta_i), \quad y_p = y_c + r_i \sin(j \Delta \theta_i) \]

\[ m_p = \rho_{mpm} r_i \Delta \theta_i \Delta R a^i \]

end for

end for
Initialization of the MPM beam pseudocode:

Input Parameters: $x_0, y_0, H, L, H_0, N_H, N_b$ (with $N_b \geq \frac{H - H_0}{2} \frac{N_H - 1}{H_0}$)

$\Delta H = \frac{H_0}{N_H - 1}$,  $L_0 = L - \frac{H - H_0}{2}$,  $N_L = \text{ceil} \left( \frac{L_0}{\Delta H} \right)$,  $\Delta L = \frac{L_0}{N_L - 1}$

#Uniform Distribution

$p = 1$

for $i = 0, ..., N_L - 1$

for $j = 0, ..., N_H - 1$

$p = p + 1$,  $x_p = x_0 + i \Delta L$,  $y_p = y_0 - \frac{H_0}{2} + j \Delta H$

$m_p = \rho_0 \Delta L \Delta H$

end for

end for

#Boundary Layers

Find $a$ such that $\sum_{k=1}^{N_b} \Delta H a^k = \frac{H - H_0}{2}$

for $i = 1, ..., N_b$

$H_i = H_0 + 2 \sum_{k=1}^{i} \Delta H a^k$,  $N_{H_i} = \text{ceil} \left( \frac{H_i}{\Delta H} \right) + 1$,  $\Delta H_i = \frac{H_i}{N_{H_i} - 1}$

$L_i = L_0 + \sum_{k=1}^{i} \Delta H a^k$,  $N_{L_i} = \text{ceil} \left( \frac{L_i}{\Delta H} \right) + 1$,  $\Delta L_i = \frac{L_i}{N_{L_i} - 1}$

for $j = 0, ..., N_{L_i} - 1$

$p = p + 1$,  $x_p = x_0 + j \Delta L_i$,  $y_p = y_0 + \frac{H_0}{2}$

$m_p = \rho_0 \Delta L_i \Delta H_i$

end for

for $j = 1, ..., N_{H_i} - 1$

$p = p + 1$,  $x_p = x_0 + L_i$,  $y_p = y_0 + \frac{H_0}{2} - j \Delta H_i$

$m_p = \rho_0 \Delta L_i \Delta H_i$

end for

for $j = 1, ..., N_{L_i} - 1$

$p = p + 1$,  $x_p = x_0 + L_i - j \Delta L_i$,  $y_p = y_0 - \frac{H_0}{2}$

$m_p = \rho_0 \Delta L_i \Delta H_i$

end for

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