

Constrained minimization problems and FFT-based solvers: application to local Dirichlet boundary conditions and contact mechanics.

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Abstract

The present paper focuses on a recent and active research axis to overcome the limitations of FFT-based solvers in order to apply various types of boundary conditions (BCs) and not only periodic BCs. A complete framework based on discrete trigonometric transforms (DTTs) of various types, possibly combined with discrete Fourier transform, has been proposed recently to account for any type of BCs defined per face of the unit-cell and per component of the displacement or traction vector. A parallel implementation by Amouzou-Adoun et al. [1] recently proved its robustness and versatility. However, this approach is not able to account for a mix of BCs on a same face (for example Dirichlet BC on a part of a face and Neumann BC on the other part of the same face), neither to prescribe Dirichlet BC to points defined inside the domain, nor to define kinematic relations between displacement on different nodes.

Starting from the displacement-based approach together with the use of DTTs, as proposed by Amouzou-Adoun et al. [1], simple modifications are proposed to account for all these questions. The modified solver, first introduced from the viewpoint of discrete local equations, is then discussed from the perspective of constrained minimization with equality constraints and the introduction of Lagrange multipliers. Simulations of a compact tension-like specimen are performed and validated. To go further, the algorithm proposed for equality constraints is then extended to account for inequality constraints to simulate contact mechanics. For the sake of validation, results obtained with a rigid spherical indenter with frictionless contact are compared to the Hertz theory for small ratios (indentation depth/sphere radius). Comparison between the small strain and finite strain context demonstrates increasing discrepancies when increasing this ratio.

It is believed that the proposed methodology will significantly expand the field of applications of FFT-based solvers.

Keywords : FFT-based solver; Lagrange multipliers; Constrained minimization; Contact Mechanics

1 : Introduction

Solving mechanical problems defined on heterogeneous unit-cells, submitted to periodic boundary conditions (BCs), with fast Fourier transform (FFT)-based algorithms was proposed initially by Moulinec and Suquet [2]. Due to their simplicity, efficiency and ability for parallelism, they have become very popular and various improvements have been proposed since the original proposition. The reader is invited to consult the review papers of Schneider [3], Lucarini et al. [4] or Gierden et al. [5], for an overview of the different advances. The next three paragraphs position our choices in terms of algorithm, spatial discretization of equations and extension to non-periodic BCs. The last paragraph introduces the central question of local Dirichlet BCs and unilateral contact, which can be regarded as constrained minimization problems. The main goal of the present paper is to introduce simple modifications in an FFT-based algorithm in order to solve these types of problems.

Regarding algorithms, the original proposition consists of a simple fixed-point algorithm [2] whose convergence strongly depends on the mechanical contrast and the choice of the reference material. To improve the efficiency of the fixed point algorithm, various propositions have been made by Eyre and Milton for the accelerated scheme [6], by Michel et al. for the Augmented Lagrangian scheme [7], and Monchiet and Bonnet for the polarization-based scheme [8]. Note that the aforementioned two methods have been recognized as special cases of the last scheme [9]. Another approach consists of switching from the fixed-point algorithm to the standard conjugate gradient algorithm, as proposed simultaneously by Zeman et al. [10] and by Brisard and Dormieux [11]. A combination of this conjugate gradient method for linear equations with a standard Newton-Raphson algorithm was then proposed, by the author [12] and Kabel et al. [13], to solve non-linear problems. In practice, since 2014 in the AMITEX_FFTP code [14] and as depicted in [15], the author accelerates the fixed-point algorithm with the same convergence acceleration technique as used in the finite element (FE) code CAST3M [16] to accelerate a modified Newton-Raphson algorithm (i.e. using a constant stiffness matrix). This implementation was recognized as an Anderson technique [17] with a depth of 4 and a periodicity of 2 or 3. In addition to an efficient convergence acceleration, with a reduced sensitivity to the mechanical contrast and to the reference material choice, it has the advantage of the quasi-Newton methods (and other solvers), not requiring the material tangent (whose implementation may be tedious). A drawback of the method is that it needs the storage of various (4 in our implementation) couples of solutions and residual fields that increases the memory footprint of the method (especially when compared to the original fixed-point algorithm).

Regarding the spatial discretization of the mechanical equations, leading to a linear system solved using Discrete Fourier Transform (DFT, abusively called FFT in the following, the Fast Fourier Transform being an efficient method used to evaluate the DFT), various approaches can be followed. The initial proposition of Moulinec and Suquet [2] can be regarded as a collocation method, starting from the continuous equation and using a truncation of Fourier series to solve the so-called Lippman-Schwinger equation for an auxiliary problem defined on a homogeneous reference material. This allows to define a Discrete Green operator (DGO) that can be applied in Fourier space using forward and backward FFT. A second approach relies on the use of variational formulations to build the DGO [18][19]. Finally, the third approach, which is adopted in the present paper, consists of using a Finite Difference (FD) scheme to build discrete differential operators (divergence, gradient) and then to build the DGO directly from the local equations. In practice the FD-based DGO is very similar to the collocation-based DGO, replacing the Fourier frequencies by “modified frequencies”, functions of the Fourier frequencies, whose definition derives from the FD scheme. An example of using a FD scheme to build the DGO in mechanical problems can be found in the work of Wiegmann in 1999 [20]. Since then, various FD schemes have been proposed and the hexahedral FD scheme (so-called “rotated scheme” by Willot

[21]) proves to be very useful in the context of mechanics of heterogeneous materials: it improves both the convergence of the solver and the quality of the solution with an efficient reduction of spurious oscillations. In addition, this hexahedral FD scheme is strictly equivalent to a hexahedral linear finite element with reduced integration [22], which allows for rigorous cross-validation as done recently in [23] for conduction problems. Quite recently, Finel proposed an alternative FD scheme based on the two symmetric tetrahedra present within a 3D voxel [24]. This novel scheme demonstrated an improvement of the stress and strain fields, solutions of elastic problems, with respect to the use of the hexahedral scheme. These two schemes are used in the present paper.

FFT-based solvers are classically written in the framework of periodicity. The question of extending the field of application of FFT-based methods from full periodic BCs to various types of BCs, has received an increasing interest in the recent years, with different proposed strategies. The first strategy relies on a buffer zone around the unit-cell so that the periodicity is applied at the boundary of the buffer [25]. This approach has been validated for both Neumann and Dirichlet BCs [26]. However, it increases the problem size and the convergence depends on the stiffness and on the thickness of the buffer (especially for Dirichlet BCs). The idea has been recently revisited by Zecevic and Lebensohn [27], using an elaborated two-level augmented Lagrangian algorithm to enforce Dirichlet BCs. A second approach consists of using symmetrized microstructures and loadings, so that Neumann or Dirichlet conditions can be applied to the unit-cell. Yet, this approach multiplies the problem size by 4 (in 2D) or 8 (in 3D) [28]. The third approach consists of taking advantage of Discrete Trigonometric (sine or cosine) Transforms (DTT) to apply whether Neumann or Dirichlet BCs. This approach was first introduced (to the authors' knowledge) in 1999 by Wiegmann [20] for homogeneous materials. Shortly, the idea was to establish the connection between Neumann, or Dirichlet, BCs and field symmetries, and to deduce from these symmetries the use of DTT (cosine or sine transform) instead of the DFT used for periodic BCs. It was then extended to heterogeneous materials, in mechanics [29], but for a limited number of "mixed" loading cases, or in conductivity for a rather exhaustive combinations of loadings, including Neumann, Dirichlet, and Periodic on each face (or couple of face for periodicity)[23]. These works were proposed in the context of FD-based DGOs. Almost in the same time, similar works have been proposed using a Galerkin approach instead of FDs [30][31][32][33][34]. Finally, the authors recently proposed a robust and efficient parallel implementation for any type of boundary condition, per face and per component, for linear and non-linear behavior, using the Small Strain and Finite Strain frameworks, based on the hexahedral and double tetrahedra FD schemes [1]. As the present work builds on this implementation, a brief description of this starting point, including algorithm, spatial discretization and DTT based non-periodic BCs, is given in section 3.

As mentioned above, using DTT allows to account for Dirichlet or Neumann or periodic BCs, per component of the displacement (or traction) vector, and per face of the unit-cell. However, the type of BC (i.e. Dirichlet, Neuman, periodic) is imposed for the whole face so that it is not possible to mix for example Neumann and Dirichlet BCs on two parts of the same face. In addition, it is neither possible to apply Dirichlet conditions to inner points of the unit-cell, nor linear relations between displacement vectors on different points. All these questions can be treated in FE codes through the introduction of Lagrange multipliers in order to solve a constrained minimization problem (equality constraint). Hence, the main goal of section 4 is to solve such problems using an efficient FFT-based solver. The proposed method has the advantage of being very simple in terms of concept and implementation. It relies on a displacement-based accelerated fixed-point algorithm, for which, at each iteration, both the kinematic conditions and the corresponding equilibrium condition are enforced. It results from a simple idea: the stress divergence is balanced by a reaction force where the displacement is prescribed. The method is first explained in sections 4.1 and 4.2, starting from the set of local discrete equations, taking into account reaction forces. In section 4.3, the method is analyzed with the viewpoint of constrained

minimization problems and the reaction forces are directly associated to Lagrangian multipliers. The application proposed in section 4.1 for testing and validating the method concerns the simulation of a half-“CT-like” specimen. Besides its prime interest for the mechanics of materials community, it requires imposing displacement at points located inside the unit-cell (to apply the loading), and, null-Neumann BC on the cracked part together with mixed Neumann/Dirichlet BC on the other part of the same face. In section 4.2, especially with the aim of reducing oscillations arising with HEX1 and TETRA2 schemes, alternative ways to apply (local) Dirichlet BCs are proposed. One of them consists of dispatching the reaction force on a set of neighboring nodes. The other one prescribes the displacement at a center of a voxel through a linear combination of the displacement at nodes. This second approach demonstrates the ability of the method to take into account linear relations between displacement at different nodes. The simulations performed in section 4, completely out of reach of standard FFT-based solvers, demonstrate the significant potential of the proposed method to widely expand the field of application of FFT-based solvers.

After considering equality constraints, the purpose of section 5 is to tackle the more complex case of minimization problems subject to inequality constraints. A typical example, once again of prime interest for the mechanics of material community, is the simulation of contact mechanics and especially of indentation. The question has already been investigated by Zecevic and Lebensohn [27] using a general approach based on a buffer layer and a rather complex algorithm (two-level augmented Lagrangian). On the other hand, many specific solvers using FFT (in 2D or 3D), devoted to contact have been investigated by the contact mechanics community (see for instance [35][36] and a review [37]). However, our goal is a bit different as we propose a quite generic FFT-based solver able to account for unilateral constraints, contact mechanics being a natural application. For the sake of simplicity, a spherical and rigid indenter is considered together with frictionless contact. The algorithm proposed in section 4 is adapted to account for a so-called active set method (the active contact zone is subject to Dirichlet constraints, i.e. sliding on the sphere surface, and the obtained solution is analyzed to detect the points where contact conditions are violated, then the active contact zone is updated and the procedure repeated until convergence). The algorithm is proposed using the Small Strain approximation or the Finite Strain framework, with minor differences to switch from one to another. To validate the method, results are compared to the Hertz theory on the reaction force as a function of the indenter depth. For small (δ (depth)/ R (indenter radius)) ratios, both the SS and FS results are very close to the Hertz theory. The stability of the results w.r.t. spatial resolution and loading discretization is then demonstrated from small to large δ/R ratios. For large δ/R ratios, the SS and FS curves depart from each other.

To summarize, section 3 briefly recalls the foundations on which the present paper relies, section 4 introduces the ability of applying equality constraints using reaction forces (i.e. Lagrange multipliers), section 5 extends section 4 to inequalities with an application to indentation. In section 4 and 5, the algorithm is first introduced from the viewpoint of local equations and then discussed from the viewpoint of constrained minimization problems. Conclusion and future prospects are proposed in section 6.

2 : Abbreviations and notations

The following abbreviations are often used in the paper: SS Small Strain, FS Finite Strain, BC Boundary Condition, IP Integration Point, VE Volume Element, FD Finite Difference, DFT Discrete Fourier Transform, DTT Discrete Trigonometric Transform, DT Discrete Transform (DTs include the DTTs and the DFT), iDFT, iDTT and iDT their inverse.

For the notations: $\mathbf{a}$ denotes a vector, $\underline{A}$ a second-order tensor, and $\mathbb{C}$ or $\mathbb{R}$ a fourth-order tensor. The divergence of a second-order tensor is $\mathbf{div}(\underline{A})$, the gradient of a vector is $\underline{\nabla}(\mathbf{a})$ and its symmetric part is $\underline{\nabla}^S(\mathbf{a})$. An index D denotes discrete divergence $\mathbf{div}_D$ or gradient $\underline{\nabla}_D$ operators (evaluated for example with a given FD scheme D).

Finally, to locate the position of multiple points in grid, the *fortran*-like (or *matlab*, or *numpy*...) notation is used. Hence the notation (0:10,10,37) refers to line of 11 nodes whose coordinates are $x_1 = 0, 1, \dots, 9, 10, x_2 = 10$ and $x_3 = 37$. This notation extends to a surface of nodes for example (0:10, 10:20,18) for 11x11 nodes. In the application below, the nodes (corners of voxels) are located at integer positions and voxel centers at half position, for example (0.5:9.5, 10.5,37.5) for the 10 voxel centers equally distributed on a line located with $x_2 = 10.5$ and $x_3 = 37.5$.

3 : FFT-based solver for periodic and non-periodic BCs

This section summarizes the choices made for the FFT-based solver used as a starting point for the extensions proposed in section 4 and 5. Its massively parallel implementation in the code AMITEX* has demonstrated its robustness through various applications in linear, non-linear, Small Strain and Finite Strain frameworks for non-trivial BCs [1]. For the sake of simplicity, the presentation builds upon the SS approximation and linear elasticity, but the extension to non-linear behaviors and FS is straightforward (see in [1]). Note that FS are also considered in section 5 to deal with contact mechanics.

3.1 : FFT-based solver with periodic BCs

3.1.1 : Problem under periodic BCs

The set of equations corresponding to a linear elastic mechanical problem, defined on a heterogeneous Volume Element Ω submitted to periodic BCs is given below in equation (1).

$$\left\{ \begin{array}{ll} \mathbf{div}(\underline{\sigma}) = 0 & \text{in } \Omega / \partial\Omega \\ \underline{\tilde{\varepsilon}} = \underline{\nabla}^S(\tilde{\mathbf{u}}) & \text{in } \Omega / \partial\Omega \\ \underline{\sigma} = \mathbb{C}: (\underline{\varepsilon}^* + \underline{\tilde{\varepsilon}}) & \text{in } \Omega / \partial\Omega \\ \tilde{\mathbf{u}}(\mathbf{x} + \mathbf{h}_d) = \tilde{\mathbf{u}}(\mathbf{x}) & \text{on opposite faces of } \partial\Omega \\ (\underline{\sigma} \cdot \mathbf{n})(\mathbf{x} + \mathbf{h}_d) = -(\underline{\sigma} \cdot \mathbf{n})(\mathbf{x}) & \text{on opposite faces of } \partial\Omega \end{array} \right. \quad (1)$$

$\underline{\sigma}$ is the second-order stress tensor, $\mathbb{C}$ the fourth-order heterogeneous elastic stiffness tensor and $\tilde{\mathbf{u}}$ the fluctuation displacement whose symmetric gradient is the fluctuation strain $\underline{\tilde{\varepsilon}}$ around an arbitrary prescribed strain field $\underline{\varepsilon}^*$ (compatible with a field $\mathbf{u}^*$, $\underline{\varepsilon}^* = \underline{\nabla}^S(\mathbf{u}^*)$). In the context of first order homogenization $\underline{\varepsilon}^*$ is generally chosen homogeneous, but it is not mandatory (see for example [38] in the context of beam or plates homogenization). The boundary conditions are explicitly defined on $\partial\Omega$ (with $\mathbf{h}_d$ the periodicity vector between two opposite faces in direction d). This description is well suited for an FE-based implementation. For an FFT-based implementation, this problem is equivalently modified into problem (2), with $\tilde{\mathbf{u}}$ and $\underline{\sigma}$ extended by periodicity.

$$\left\{ \begin{array}{ll} \mathbf{div}(\underline{\sigma}) = 0 & \text{in } \Omega^\infty \\ \underline{\tilde{\varepsilon}} = \underline{\nabla}^S(\tilde{\mathbf{u}}) & \text{in } \Omega^\infty \\ \underline{\sigma} = \mathbb{C}: (\underline{\varepsilon}^* + \underline{\tilde{\varepsilon}}) & \text{in } \Omega \\ \tilde{\mathbf{u}} & \Omega - \text{periodic} \quad \text{in } \Omega^\infty \\ \underline{\sigma} & \Omega - \text{periodic} \quad \text{in } \Omega^\infty \end{array} \right. \quad (2)$$

Using extended fields, the derivation (of $\tilde{\mathbf{u}}$ or $\underline{\sigma}$) around a point located at the boundary $\partial\Omega$ is the same as around any other point in the volume Ω . Considering a regular grid discretization, discrete derivation is then invariant by translation and can be evaluated using Discrete Fourier Transform.

In the following, the spatial discretization of Ω is considered with a regular grid of cubic elements, or voxels (for simplicity, but a grid of parallelepiped elements can be considered as well), with displacement $\tilde{\mathbf{u}}^i$ and $\mathbf{div}(\underline{\sigma})^i$ defined at nodes i , and stress $\underline{\sigma}^i$ and strain $\underline{\varepsilon}^i$ defined at integration points of element i . For more than a single integration point, this simplified notation $\underline{\sigma}^i$ gathers the stress evaluated at all the integration points of element i . In the present paper, focus is put on the discrete derivation schemes HEX1 corresponding to linear FE with a single IP [21][22], and the TETRA2 scheme recently proposed by Finel [24] (and described in a more simple and practical way in [39]), with 2 IPs defined at the center of each element (i.e. voxel). For each IP, the strain is deduced from the displacement of nodes located on one of the two tetrahedra defined from the 8 nodes of the cube (see Figure 1).

For the sake of simplicity, exponent i is omitted unless necessary (as in section 4 where displacement is prescribed on specified nodes).

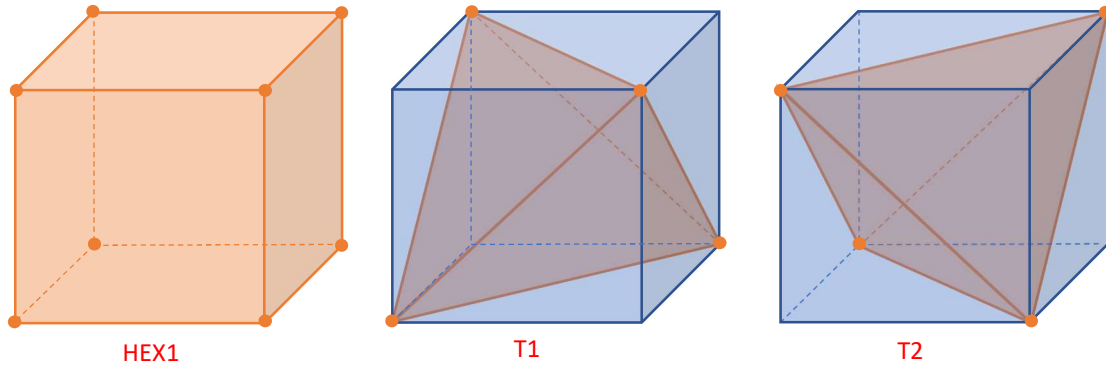


Figure 1 : Description of the HEX1 and TETRA FD schemes. For the HEX1 scheme, displacement gradient is evaluated at a single integration point (center of the voxel), and for the TETRA2 scheme, two gradients are evaluated at two IPs located at voxel center, each value associated to one of the two tetrahedra T1 and T2.

3.1.2 : Discrete Green operator and fixed-point algorithm.

Considering the discretized equations, the periodic extension used in problem (2), and introducing the term $\mathbb{R}_0 : \underline{\nabla}_D(\tilde{\mathbf{u}})$, problem (2) can be re-written as problem (3) - left part.

$$\begin{cases} \underline{\sigma} = \mathbb{C} : (\underline{\varepsilon}^* + \underline{\nabla}_D^s(\tilde{\mathbf{u}})) \\ \mathbf{p} = \mathbf{div}_D(\underline{\sigma} - \mathbb{R}_0 : \underline{\nabla}_D(\tilde{\mathbf{u}})) \\ \mathbf{div}_D(\mathbb{C}_0 : \underline{\nabla}_D^s(\tilde{\mathbf{u}})) = -\mathbf{p} \end{cases} \quad \Leftrightarrow \quad \begin{cases} \underline{\sigma} = \mathbb{C} : (\underline{\varepsilon}^* + \underline{\nabla}_D^s(\tilde{\mathbf{u}})) \\ \mathbf{p} = \mathbf{div}_D(\underline{\sigma} - \mathbb{R}_0 : \underline{\nabla}_D(\tilde{\mathbf{u}})) \\ \hat{\tilde{\mathbf{u}}} = \hat{\mathbb{G}}_D(\hat{\mathbf{p}}) \end{cases} \quad (3)$$

Here, $\mathbb{R}_0$ is a fourth-order tensor, generally associated with an isotropic behavior (this is no more the case for general non-periodic BCs, see section 3.2.3). In addition, a subscript D has been added to derivation operators, $\mathbf{div}$ and $\underline{\nabla}$, in order to emphasise the discrete derivation and, consequently the discrete nature of these equations. In the present paper, D corresponds to the HEX1 or TETRA2

scheme. For these two schemes, the discrete displacement and stress divergence fields are defined at voxel corners (nodal fields) and the stress and displacement gradients at voxel centers (element fields).

Solving problem (3) - left part, assuming periodic extensions of $\tilde{\mathbf{u}}$ and $\underline{\sigma}$, can be done using Discrete Fourier Transform (with the notation $DFT(f) = \hat{f}^{DFT}$ or simply $\hat{f}$) as depicted in problem (3) - right part, that defines the following fixed-point algorithm: first step, for a given $\tilde{\mathbf{u}}$ evaluate $\underline{\sigma}$ and then $\mathbf{p}$ in real space, second step, evaluate a new $\tilde{\mathbf{u}}$ from the application of the discrete Green operator $\mathbb{G}_D$ (using a back and forth in Fourier space), and iterate until convergence. This displacement-based algorithm requires the evaluation of gradient and divergence in real space (using HEX1 or TETRA2 scheme), which is quite different from the strain-based algorithm originally proposed in [2] and still widely used. Note that working with the displacement field as unknown, instead of the strain field, simplifies the application of local Dirichlet BC in section 4.

For the HEX1 scheme, using an isotropic elastic behavior for $\mathbb{R}_0$, with Lamé coefficients (λ_0, μ_0) , the expression of the discrete Green operator in Fourier space reads:

$$\hat{\mathbf{u}} = \mathbb{G}_D(\hat{\mathbf{p}}) = -\frac{\hat{\mathbf{p}}}{\mu_0 \|\xi_D\|^2} + \frac{(\lambda_0 + \mu_0) \hat{\mathbf{p}} \cdot \xi_D}{(\lambda_0 + 2\mu_0) \|\xi_D\|^4} \xi_D \quad (4)$$

In this equation, ξ_D represents the modified wave vectors associated to the HEX1 scheme (D=HEX1). As well as $\hat{\mathbf{u}}$ and $\hat{\mathbf{p}}$, ξ_D is defined on a 3D grid discretizing the Fourier space, with the same grid size as the grid in physical space (in practice, as the physical fields are real-valued, the 3D-DFT only stores a half of the grid in Fourier space, generally the first direction is reduced). This equation is evaluated locally at each point of Fourier space. The expression of ξ_D can be found in [21] for the HEX1 scheme. The expression of the discrete Green operator is a bit more complex for the TETRA2 scheme and can be found in [24] and [1].

To improve the convergence of the fixed-point algorithm, the convergence acceleration technique proposed by the developers of the CAST3M FE-code to accelerate the modified-Newton Raphson algorithm for solving non-linear problems [16] is directly applied to the fixed-point algorithm. This acceleration convergence technique was identified as an Anderson convergence acceleration method [40].

Finally, the convergence criteria used to stop the iterative algorithm is evaluated on the equilibrium condition. It reads for cubic voxels of size h (an expression is proposed in [26] for non-cubic voxels):

$$\frac{h \|\mathbf{div}_D(\underline{\sigma})\|_2}{\|\underline{\sigma}\|_2} < tol_{eq} \quad (5)$$

To sum-up, this section provides a quick overview of the FFT-based solver used in the present paper. If the use of a displacement-based algorithm, with evaluation of derivatives in real space, can be regarded as an originality also described in a recent companion paper [1], the other aspects are rather standard and can be found in review articles focused on FFT-based solvers [3][4].

3.2 : Extension to non-periodic BC using DTTs

Recently, the question of the extension of FFT-based solvers to non-periodic BCs has been addressed by several teams, using appropriate Discrete Trigonometric Transforms instead of a Discrete Fourier Transform in each direction for each component of the displacement or traction vector [23][41][34]. This approach allows to apply whether Neumann or Dirichlet or periodic BCs on each face and for each component of the displacement/traction vector. The purpose of the present section is to give an overview of this approach, the interested reader is invited to read [1] to go deeper into details.

3.2.1 : Correspondence between boundary conditions and symmetry extensions

First of all, the problem to solve is the same as problem (1) except the boundary conditions. In the general case, for each face, each component of the displacement or traction vector is submitted to whether Neumann, Dirichlet or periodic BCs (considering couple of opposite faces in case of periodic BC). As in the previous section, the first step consists in replacing the problem with boundary conditions (similar to problem (1)) by a problem with appropriate field extensions for the fluctuation displacement $\tilde{\mathbf{u}}$ and stress $\underline{\sigma}$ (similar to problem (2)). In the case of null-Neumann or Dirichlet conditions, the extensions are symmetries: even-symmetry (S for Symmetry) or odd-symmetry (A for Antisymmetry). Hence, the problem can be written in the most general case as follows:

$$\begin{cases} \mathbf{div}(\underline{\sigma}) = 0 & \text{in } \Omega^\infty \\ \underline{\varepsilon} = \underline{\nabla}^s(\tilde{\mathbf{u}}) & \text{in } \Omega^\infty \\ \underline{\sigma} = \mathbb{C} : (\underline{\varepsilon}^* + \underline{\varepsilon}) & \text{in } \Omega \\ \tilde{\mathbf{u}} \text{ appropriate symmetries} & \text{in } \Omega^\infty \\ \underline{\sigma} \text{ appropriate symmetries} & \text{in } \Omega^\infty \end{cases} \quad (6)$$

The question is now to define the “appropriate symmetries”. For that purpose, the 6 faces bounding the Volume Element are denoted S_J^0 and S_J^1 ($J = 1:3$): S_J^0 with an outer normal vector $\mathbf{N}_J^0 = -\mathbf{e}_J$, positioned at $x_J = 0$, and S_J^1 positioned at $x_J = L_J$ with an outer normal $\mathbf{N}_J^1 = \mathbf{e}_J$. The appropriate symmetries of $\tilde{\mathbf{u}}$ and $\underline{\sigma}$ can be completely determined according to Table 1, considering each component i and each face S_J^α .

	$\tilde{u}_i$	σ_{ij}	$\sigma_{ij} (j \neq J)$
Dirichlet	A	S	A
Neumann	S	A	S
Periodicity	P	P	P

Table 1: Extensions used to satisfy Dirichlet, Neumann or Periodic condition for component i on a face S_J^α (A for Antisymmetry (odd-symmetry), S for even-symmetry, and P for periodicity)

To clarify the idea behind this table, it must be noted that an odd-symmetry (A) enforces a field to vanish at boundary and, conversely, an even-symmetry (S) let the quantity free (unconstrained) at boundary. Hence, for Dirichlet condition on component i on a face S_J^α , the extension of $\tilde{u}_i$ is A (imposed null) and σ_{ij} is S (free). Using the symmetries proposed for the other components of $\underline{\sigma}$ in the last column of Table 1, it can be verified that the component i of $\mathbf{div}_D(\underline{\sigma})$ systematically vanishes at the boundary (extension of $(\mathbf{div}_D(\underline{\sigma}))_i$ is A). In other words, as the component i of the unknown fluctuation displacement is imposed at the boundary, by construction (using symmetry extensions), the corresponding equilibrium equation is eliminated, by construction. On the other hand, for null-Neumann condition on component i on a face S_J^α , the extension of σ_{ij} is A (imposed null) and $\tilde{u}_i$ is S (free). Using the symmetries proposed in Table 1, the component i of $\mathbf{div}_D(\underline{\sigma})$ is let completely free (extension of $(\mathbf{div}_D(\underline{\sigma}))_i$ is S). In other words, the component i of the unknown fluctuation

displacement is let free at the boundary, by construction (using symmetry extensions), and the corresponding equilibrium equation is fully active (i.e. not imposed to zero by construction).

3.2.2 : Correspondence between symmetry extensions and DTTs

In section 3.1, a discrete transform, the Discrete Fourier Transform, is associated to a periodicity extension. Here, a Discrete Trigonometric Transform is associated to a symmetry extension (whether S or A on opposite faces). The corresponding association is given in Table 2 below, using the same designation as in the *fftw* library [42] for Discrete Sine and Cosine Transforms).

Symmetries	Nodal field ($\tilde{\mathbf{u}}$)	Element field ($\underline{\sigma}$)
SS	DCT1	DCT2
SA	DCT3	DCT4
AA	DST1	DST2
AS	DST3	DST4

Table 2 : Correspondence between symmetries on opposite faces and the appropriate Discrete Trigonometric Transform

Note that this correspondence table assumes that boundary nodes coincide with the faces of the VE, and, consequently, that voxel centers do not. As $\tilde{\mathbf{u}}$ is a nodal field and $\underline{\sigma}$ is an element field defined at voxel centers, their corresponding DTTs differ. In practice, DTTs are only applied to nodal fields for the algorithm proposed in the present paper.

3.2.2 : Correspondence between DTTs and DFT

The last important ingredient for this extension to non-periodic BCs lies in the relationship between DTTs applied to the current cell and DFT applied on extended cells. This relation can be written when considering 4-times extended cells following equation (7) together with Table 3 below.

$$S_{4F}(\widehat{q_4}) = \alpha DTT(S_R(q)) \quad (7)$$

DTT	S_R : selection in $[0:n]$ (Real space)	S_{4F} : selection in $[0:4n-1]$ (Fourier space)	N : number of selected points	α
DCT1	$[0:n]$	$2 \times [0:n] \quad (0,2,4, \dots, 2n)$	$n+1$	2
DCT3	$[0:n-1]$	$2 \times [0:n-1] + 1 \quad (1,3,5, \dots, 2n-1)$	n	2
DST1	$[1:n-1]$	$2 \times [1:n-1] \quad (1,3,5, \dots, 2n-1)$	$n-1$	$-2i$
DST3	$[1:n]$	$2 \times [0:n-1] + 1 \quad (0,2,4, \dots, 2n)$	n	$-2i$

Table 3 : Selection of points in real space (to be used as input of DTTs) and selection of points in Fourier space for the 4 times extended signals.

Equation (7) deals with a nodal signal q (i.e. a component of $\tilde{\mathbf{u}}$ or $\mathbf{p}$ (see definition in equation (3)), which can be extended using the appropriate symmetries (see correspondence Table 2) to define a 4-times larger signal q_4 that is periodic on which DFT can be applied to obtain $\widehat{q_4} = DFT(q_4)$. The signal q being defined on $[0:n]$ (i.e. $n+1$ points), DTT is applied to a selected subset of q defined by S_R , a selection operator. In practice, the points concerned by an antisymmetry condition are not selected (for example with DST3, corresponding to symmetry AS, the first point is not selected and S_R selects the subset $[1:n]$). Finally, equation (7) exhibits that, up to a factor α , each point of the DTT signal corresponds to a specific selected point in the DFT of the 4-times extended signal. The selection operator S_{4F} acting on the DFT of the extended signal is given in Table 3.

3.2.3 : Application of the discrete Green operator

An important point when dealing with non-periodic BCs through DTTs is that the usual reference material $\mathbb{R}_0$ (with $\mathbb{R}_0:\nabla\mathbf{u} = \lambda_0 \text{Tr}(\nabla\mathbf{u})\mathbf{I} + 2\mu_0\nabla^S\mathbf{u}$) associated with an isotropic elastic stiffness tensor can only be used for a limited set of BCs corresponding to periodic and normal mixed BCs (see for instance [34], [41] or [1]). In the most general case, one can use $\mathbb{R}_0:\nabla\mathbf{u} = 2\mu_0\nabla\mathbf{u}$ or, as proposed by Paux et al. [34], $\mathbb{R}_0:\nabla\mathbf{u} = \lambda_0\nabla\mathbf{u}\odot\mathbf{I} + 2\mu_0\nabla\mathbf{u}$ (with $\odot$ the Hadamard product, so that $(\underline{A}\odot\underline{B})_{ij} = A_{ij}B_{ij}$, no summation on indices). In the different applications proposed in the present paper, this last proposition is kept.

Finally, the discrete Green operator defined for periodic boundary conditions (see equation (4), to be adapted according to the choice on $\mathbb{R}_0$ just above) can be used as well on the 4-times extended signal (periodic). Importantly, the application of the discrete Green operator is never evaluated on the complete DFT of the 4-times extended signal but only to the points selected by S_{4F} . Fields are ‘virtually’ extended but the extensions are never stored in memory.

3.2.4 : Consequences on the algorithm and its implementation

As a consequence, from an algorithm point of view, the fixed-point defined by the 3 successive steps corresponding to each line of problem (3)-right part, is exactly the same for non-periodic BCs and the convergence acceleration can be applied identically. The most important differences concern the application of different types of DT (or iDT) (possibly different for each component (of $\tilde{\mathbf{u}}$) and for each direction) on a carefully selected subset (S_R selection), and inversely, the application of inverse DTTs on $S_{4F}(\widehat{\mathbf{p}}_4)$ taking care of the S_R selection to obtain $\mathbf{p}$. In addition, it must be noticed that combining periodic and non-periodic boundary conditions, the components (of $\tilde{\mathbf{u}}$ or $\mathbf{p}$) in Fourier space can be purely real (if non-periodic in the 3 directions) or complex (if at least one direction is submitted to periodicity). In that second case, as the input field is real, the size of the transformed field is half-sized in the direction of the first periodicity condition. Hence, the implementation must handle fields in Fourier space having, for each component, possibly different types (real and complex), and for complex components, possibly different shapes. Implementation details can be found in [1], especially for a massively parallel (distributed memory) implementation using the *2decomp&fft* library [43] enhanced for that purpose.

To summarize, the extension of FFT-based solvers to non-periodic BCs through the use of DTTs (instead of DFT for non-periodic BCs) is not conceptually complicated but the implementation in the most general case requires a careful attention. Such an implementation was performed as a partial re-writing of the massively parallel code AMITEX [14] into a new version AMITEX*, implemented for linear and non-linear behaviors, in the small and finite strains framework [1].

However, if it greatly expands the field of application of FFT-based solvers, the limitation of this approach is that the type of condition (Neumann, Dirichlet or periodic) is homogeneous per face: it is not possible to mix Dirichlet condition on a part of a face and Neumann on the other part of the same face. The second limitation is that the conditions are applied at the faces of the VE but cannot be applied inside the VE. As FFT-based solvers are defined on grids, it can be useful to apply Dirichlet conditions in the VE: a typical example proposed in the present paper concerns the simulation of a Compact Tension (CT)-like specimen (a simplified version of a Compact Tension specimen).

4 : Local Dirichlet conditions – Minimization under equality constraints

Using DTT in addition to FFT, as summarized in the previous section, allows to significantly extend the field of applications of FFT-based solvers (once again, DTTs can be regarded as an FFT on a larger cell and the designation FFT-based solver is kept). However, this extension still suffers a limitation: if the type of BC, whether Neumann, Dirichlet or periodicity depends on the component of the displacement or traction vector, it must be the same for all the points belonging to a given face of the VE. Hence, it is not possible to have a surface free almost everywhere but with prescribed displacement on some few points, lines or areas (as classically done in standard FE solvers), nor to apply displacements at interior points within the VE. Such capabilities will open the door of structural analysis to FFT-based solver, with the advantage for the user to take benefit of massively parallel implementations. The approach for prescribing local Dirichlet BC whether at free surface or in the volume is introduced below. A first proposition is made to apply strongly the local BCs, however it appears to be not well-suited to TETRA2 or HEX1 elements, giving rise to important oscillations. To circumvent this issue, two options are proposed to relax the first proposition and vanish oscillations. Finally, the method described with the viewpoint of local equations is regarded from the perspective of minimization problem under equality constraints associated to the introduction of Lagrange multipliers.

4.1 : Strongly applied conditions

4.1.1: Method and algorithm

The first proposition consists in applying strongly the Dirichlet conditions on a given set of nodes I_0 in directions gathered in the set J_0 (i.e. each element $I_0(k) = i_0$ is a node number, and each corresponding element of $J_0(k) = j_0$ is an integer between 1 and 3, representing the prescribed direction for node i_0). The prescribed displacements are denoted $(\mathbf{U}^{I_0})_{J_0}$. Assuming the existence of reaction forces acting, as consequence of the applied displacement, on the same nodes and in the same directions, denoted $(\mathbf{f}^{I_0})_{J_0}$, the equations of the problem are given below.

$$\begin{cases} \mathbf{div}(\underline{\sigma}) + (\mathbf{f}^{I_0})_{J_0} = 0 & \text{in } \Omega^\infty \\ \underline{\tilde{\varepsilon}} = \underline{\nabla}^s(\tilde{\mathbf{u}}) & \text{in } \Omega^\infty \\ \underline{\sigma} = \mathbb{C} : (\underline{\tilde{\varepsilon}}) & \text{in } \Omega \\ (\tilde{\mathbf{u}}^{I_0})_{J_0} = (\mathbf{U}^{I_0})_{J_0} \\ \tilde{\mathbf{u}} \text{ appropriate symmetries} & \text{in } \Omega^\infty \\ \underline{\sigma} \text{ appropriate symmetries} & \text{in } \Omega^\infty \end{cases} \quad (8)$$

For the sake of simplicity, it is assumed that $\mathbf{u}^*$, and consequently $\underline{\varepsilon}^*$, is set to zero so that the displacement condition is directly applied to $\tilde{\mathbf{u}}$. Definition of “appropriate symmetries” refers to the previous section and corresponds to Neumann or Dirichlet or periodic conditions applied on the 6 faces. Note that the local Dirichlet conditions are applied whether on interior nodes or on nodes of the faces on which null-Neumann conditions are applied. In addition, we assume that “enough” Dirichlet BCs are applied through symmetry extensions to remove any free rigid body motion. To solve this problem, the fixed-point algorithm defined by the set of successive equations (9) is proposed.

$$\begin{cases} proj_U : (\tilde{\mathbf{u}}^{I_0})_{J_0} = (\mathbf{U}^{I_0})_{J_0} \\ \underline{\sigma} = \mathbb{C} : (\underline{\nabla}_D^s(\tilde{\mathbf{u}})) \\ \mathbf{p} = \mathbf{div}_D(\underline{\sigma}) \\ proj_P : (\mathbf{p}^{I_0})_{J_0} = 0 \\ \mathbf{p} = \mathbf{p} - \mathbf{div}_D(\mathbb{R}_0 : \underline{\nabla}_D(\tilde{\mathbf{u}})) \\ \hat{\tilde{\mathbf{u}}} = \hat{\mathbb{G}}_D(\hat{\mathbf{p}}) \end{cases} \quad (9)$$

The differences with the algorithm described in problem (3)-right part are minor and correspond to the addition of the lines referenced $proj_U$ and $proj_P$. Line $proj_U$ is the projection of the current fluctuation field $\tilde{\mathbf{u}}$ on the space of kinematically admissible fields (i.e. simply set the prescribed displacements) and line $proj_P$ is the projection of the current residual field $\mathbf{p}$ on the set of statically admissible fields (i.e. simply set $(\mathbf{div}(\underline{\sigma})^{I_0})_{J_0} + (\mathbf{f}^{I_0})_{J_0} = 0$). In other word, where the displacement is imposed the stress divergence is systematically balanced by a reaction force to satisfy equilibrium. Note that the reaction forces $(\mathbf{f}^{I_0})_{J_0}$ can be evaluated as a post-treatment, once convergence achieved.

Remark: The reaction forces $(\mathbf{f}^{I_0})_{J_0}$ correspond to the definition of the Lagrange multipliers commonly introduced to apply Dirichlet BC in FE direct solvers (see section 4.3). In these solvers, the Lagrange multipliers are added to the vector of nodal unknowns (in addition to the vector of nodal displacements), and the system to be solved is enlarged accordingly. In the present proposition, the same iterative solver as introduced in section 3 (i.e. an accelerated fixed-point algorithm), is used with minor modifications that simply consists of a projection of the displacement field ($\tilde{\mathbf{u}}$, forcing displacements to fulfil Dirichlet conditions) and a projection of the residual field ($\mathbf{p}$).

The algorithm is detailed below with emphasis on the parts added to the classical fixed-point algorithm written in black (see Algorithm 1). In blue, the convergence accelerations parts are depicted. Note that the recent proposition [1] allows to accelerate whether the displacement field $\tilde{\mathbf{u}}$, if ACV_U is true, or the quantity $\mathbf{p} - \mathbf{div}_D(\mathbb{R}_0 : \underline{\nabla}_D(\tilde{\mathbf{u}}))$, if ACV_P is true. In practice, the function ACV_{storeR} stores the residual fields (difference between two successive solutions, i.e between the end and the beginning of the iteration) while ACV_{storeS} stores the corresponding solution fields (at the beginning of the iteration). The two corresponding tables have four indices and the fields are stored at each iteration using cycling indices. After the four first iterations and every mod_{ACV} iterations (generally 2 or 3), an accelerated solution can be proposed from the four solution and residual fields stored in the tables (following an Anderson acceleration technique described in [15] in the context of FFT-based solvers).

```

1. Initial  $\tilde{\mathbf{u}} = \mathbf{0}$ 
2.  $proj_U : (\tilde{\mathbf{u}}^{l_0})_{J_0} = (\mathbf{U}^{l_0})_{J_0}$ 
3. Loop  $i \geq 0$ 
4.   if ( $ACV_U$ )
5.     if ( $i > 0$ )  $ACV_{storeR}(i, \tilde{\mathbf{u}})$ 
6.     if ( $i > 0$  & modulo( $i, mod_{ACV}$ ) = 0)  $ACV_{accelerate} \rightarrow \tilde{\mathbf{u}}$ 
7.      $ACV_{storeS}(i, \tilde{\mathbf{u}})$ 
8.      $\underline{\sigma} = \mathbb{C} : \nabla_D^s(\tilde{\mathbf{u}})$ 
9.      $\mathbf{p} = \mathbf{div}_D(\underline{\sigma})$ 
10.     $proj_P : (\mathbf{p}^{l_0})_{J_0} = \mathbf{0}$ 
11.    if equilibrium( $\mathbf{p}$ ): EXIT Loop
12.     $\mathbf{p} = \mathbf{p} - \mathbf{div}_D(\mathbb{R}_0 : \nabla_D(\tilde{\mathbf{u}}))$ 
13.    if ( $ACV_P$ )
14.      if ( $i > 0$ )  $ACV_{storeR}(i, \tilde{\mathbf{p}})$ 
15.      if ( $i > 0$  & modulo( $i, mod_{ACV}$ ) = 0)  $ACV_{accelerate} \rightarrow \tilde{\mathbf{p}}$ 
16.       $ACV_{storeS}(i, \tilde{\mathbf{p}})$ 
17.       $DT(\mathbf{p}) \rightarrow \hat{\mathbf{p}}$ 
18.       $\hat{\tilde{\mathbf{u}}} = \mathbb{G}_D(\hat{\mathbf{p}})$ 
19.       $iDT(\hat{\tilde{\mathbf{u}}}) \rightarrow \tilde{\mathbf{u}}$ 
20.     $proj_U : (\tilde{\mathbf{u}}^{l_0})_{J_0} = (\mathbf{U}^{l_0})_{J_0}$ 

```

Algorithm 1 : Description of the FFT-based algorithm proposed to account for local kinematic constraints (Dirichlet constraints) defined at nodes. In black, the lines corresponding to the standard fixed-point algorithm, in blue, the convergence acceleration (whether on $\tilde{\mathbf{u}}$ if ACV_U is true, or on $\mathbf{p} - \mathbf{div}_D(\mathbb{R}_0 : \nabla_D(\tilde{\mathbf{u}}))$ if ACV_P is true) and, in red, the lines proposed to apply the constraints.

To sum up, compared to the displacement-based algorithm recently proposed in [1], accounting for non-periodic BCs through DTTs, the introduction of local displacement constraints is very simple (see red lines in Algorithm 1). This algorithm is tested and validated below on a CT-like specimen associated to a loading case out of reach for standard FFT-based solvers (periodic) and even to non-periodic solvers based solely on DTTs.

4.1.2: Results on CT-like specimen

The CT-like specimen is both interesting for the mechanics of material community and challenging for the FFT-based solvers community. Actually, in addition to non-periodic boundary conditions with Neumann and Dirichlet on a same face, together with Dirichlet on interior points, the proposed simulation has the originality of simulating an accurate crack (instead of a crack with a one voxel thickness). The description of the simulated unit-cell is proposed on Figure 2. This setup comes after different unfruitful attempts when trying to apply null-Neumann on the 6 faces and constraints on local vertical displacement (on the red line and surface). To overcome this issue, it is proposed to use a void buffer layer (green on Figure 2) that allows for applying Dirichlet condition (vertical) on face S_3^0 (yellow face on Figure 2), null-Neumann on the other faces, and local constraints on the vertical displacement on red line and surface. Boundary conditions on faces are applied using symmetry extensions (through DTTs) and local constraints are applied using the proposed strategy in Algorithm 1.

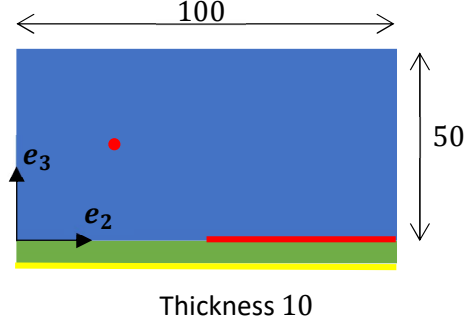


Figure 2: Half CT-like specimen description: the blue part represents the half CT specimen, the green part a void buffer layer (1 voxel thickness), the red dot represents the projection along the direction $\mathbf{e}_1$ of the line (position $(0:10,25,25)$), which is subjected to a displacement of 10 in direction $\mathbf{e}_3$ (vertical), the red line the projection along the direction $\mathbf{e}_1$ of the surface (position $(0:10,50:100,0)$), which is subjected to a null displacement in direction $\mathbf{e}_3$ (vertical) and the yellow surface $(0:10,0:100,-1)$ is subjected to a null displacement in direction $\mathbf{e}_3$ (vertical).

The used discretization is $10 \times 100 \times (50+1)$ voxels with a single voxel of void layers (green). The void layer is considered as an elastic material with null properties and the CT-like specimen material is elastic isotropic with $(4.04 \cdot 10^4, 2.70 \cdot 10^4) \text{ GPa}$ for the Lamé coefficients (λ, μ) . The discrete Green operator is defined with the $\mathbb{R}_0$ tensor proposed by Paux et al. [34] for general non-periodic BCs (see section 3.2.3) using $(\lambda_0, \mu_0) = (\lambda/2, \mu/2)$. All the results presented below have been obtained using the TETRA2 finite derivation scheme (simulations with HEX1 scheme did not converge).

In spite of a simulation expected quite complex for FFT-based solvers, it must be noticed that convergence is achieved without any particular issue using convergence acceleration (it fails without). As observed in Table 1 the new proposition ACV_P exhibits a better convergence and the best choice is obtained with $mod_{ACV} = 2$.

	$mod_{ACV} = 2$	$mod_{ACV} = 3$
ACV_U	399	539
ACV_P	198	321

Table 1: Number of iterations at convergence with different choices of convergence acceleration (convergence tolerance 10^{-4} , using TETRA2 elements). With ACV_U , acceleration is applied to fluctuation displacement fields, with ACV_R acceleration is applied to the field $\mathbf{p} - \text{div}_D \left(\mathbb{R}_0 : \nabla_D(\tilde{\mathbf{u}}) \right)$ (see Algorithm 1).

A representation of the deformed configuration together with the stress field σ_{33} in Figure 3 (– top), shows the ability of the FFT-based solver to reproduce this CT-like simulation. It must be emphasized that no spurious oscillations can be observed on the two representations (deformed shape and stress field), demonstrating the ability of the TETRA2 scheme to produce smooth results (note that the represented stress field is evaluated on one of the two integration points, it is not an average over the two IPs that could have reduce oscillations). The other results in Figure 3 (– middle and bottom) correspond to the loading applied “weakly” with the TETRA2 scheme (– middle) and the HEX1 scheme (– bottom), as proposed in the following section 4.2.

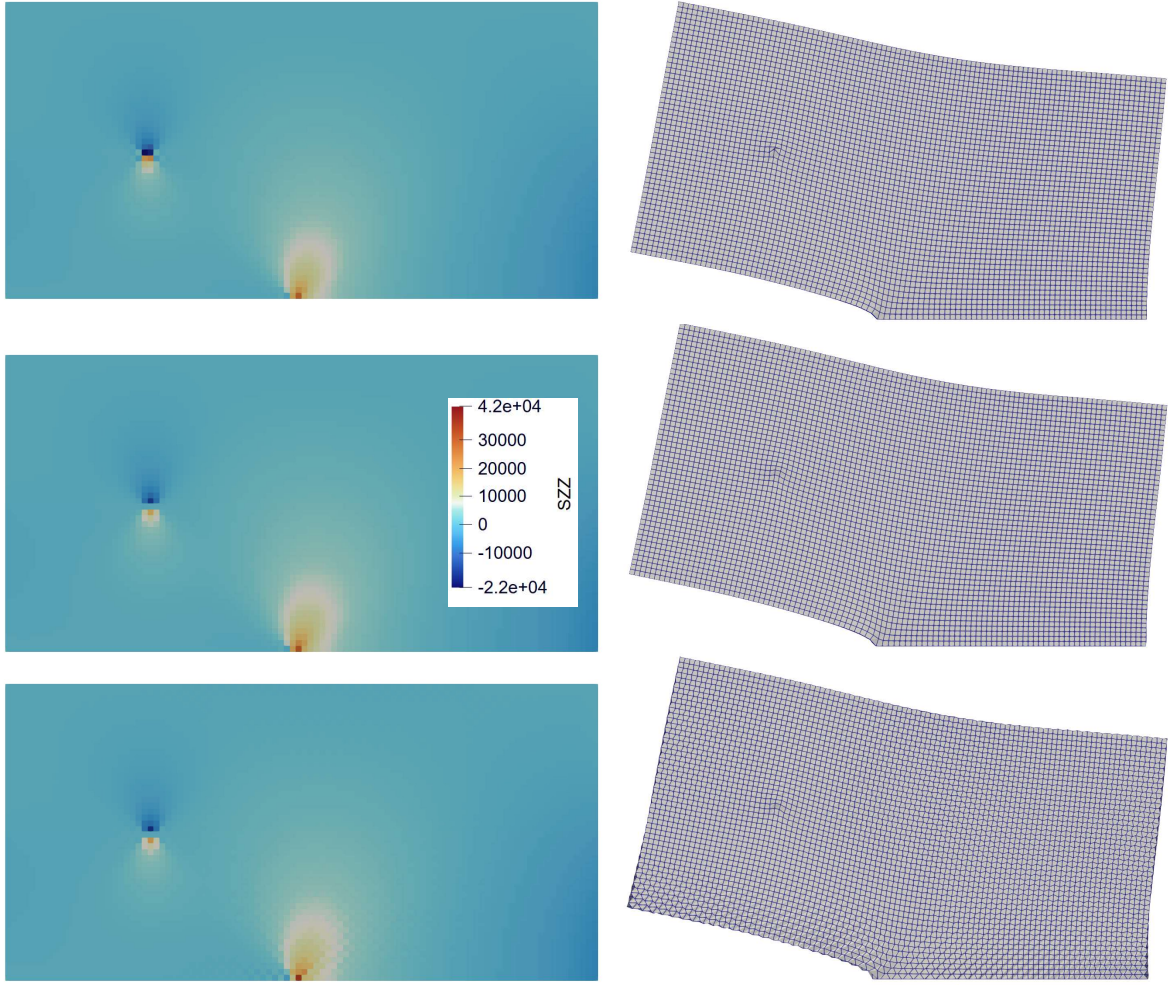


Figure 3: Representation (buffer layer removed) of the deformed configuration and σ_{33} stress field (on one of the two integration points) for three simulations: (top) TETRA2 elements with displacement strongly applied on the line of nodes (0:10,24,24), (middle) TETRA2 elements with displacement applied weakly to the line of elements (0.5:9.5,24.5,24.5), (bottom) HEX1 elements with displacement applied weakly to the line of elements (0.5:9.5,24.5,24.5). See section 4.2.1 for the meaning of “displacement applied weakly”.

4.1.3 : Validation

The procedure for applying local Dirichlet BC is validated from a cross-comparison with the same simulation performed with the FE code CAST3M [16] that uses a direct solver. The two simulations have the same regular mesh, the same material parameters and the same loading as described in the previous section. The only difference is the type of element: linear hexahedral elements with full integration (8 integration points) for the FE simulation and TETRA2 elements for the present FFT-based simulation. For this comparison between a direct and an iterative solver, the tolerance of the iterative FFT-based solver (see equation (5)) is lowered to 10^{-1} . The equilibrium criterion is reached after 576 iterations. The comparison is made between vertical stress field (σ_{33}), using the value interpolated at the center of the element for the FE simulation and the average of the two values for the TETRA2 element (i.e. one value for each tetrahedra of a same voxel). In addition, the resultant reaction forces R_s and R_L are respectively evaluated on the surface of nodes located at the crack tip subject to null vertical displacement $\tilde{u}_3$, and on the line of nodes on which the opening displacement $\tilde{u}_3$ is prescribed. Note that for the FFT-based simulation, due to boundary symmetries, the value of the reaction is

divided by 2 for nodes located at a boundary face and by 4 for nodes located at corners between two boundary faces. Interestingly, it is observed that the macroscopic equilibrium condition $R_S + R_L = 0$ is not met at the beginning of the iterative algorithm but is almost reached at convergence with a relative error of $5 \cdot 10^{-12}$ (i.e. $(|R_S| - |R_L|)/|R_L|$ with $|R_S| = 8418.91935121 \text{ N}$ and $|R_L| = 8418.91935126 \text{ N}$). When comparing the norm of the reactions for the FE simulation ($|R_L^{FE}| = 8505.04 \text{ N}$) and the present FFT-based simulation ($|R_L^{FFT}| = 8418.92 \text{ N}$), the relative error, $(|R_L^{FFT}| - |R_L^{FE}|)/|R_L^{FE}|$, is $1.02 \cdot 10^{-2}$ ($\sim 1\%$). This quantitative comparison is extremely satisfying if we consider that the two simulations have been run with different types of elements and a moderate discretization. To further explore this comparison, stress fields on two different planes are displayed in Figure 4. This qualitative comparison between the FE simulation (upper image in Figure 4) and the FFT-based simulation (lower image in Figure 4) exhibits a very nice agreement. The most important differences are observed at the crack tip and around the loading line, but they remain limited. It can be noticed that the particular shape of the stress field at the crack type in the (e_1, e_2) plane is also reproduced (the stress field is not invariant in the e_1 direction). As a conclusion, this cross-comparison validates the proposed method and its implementation.

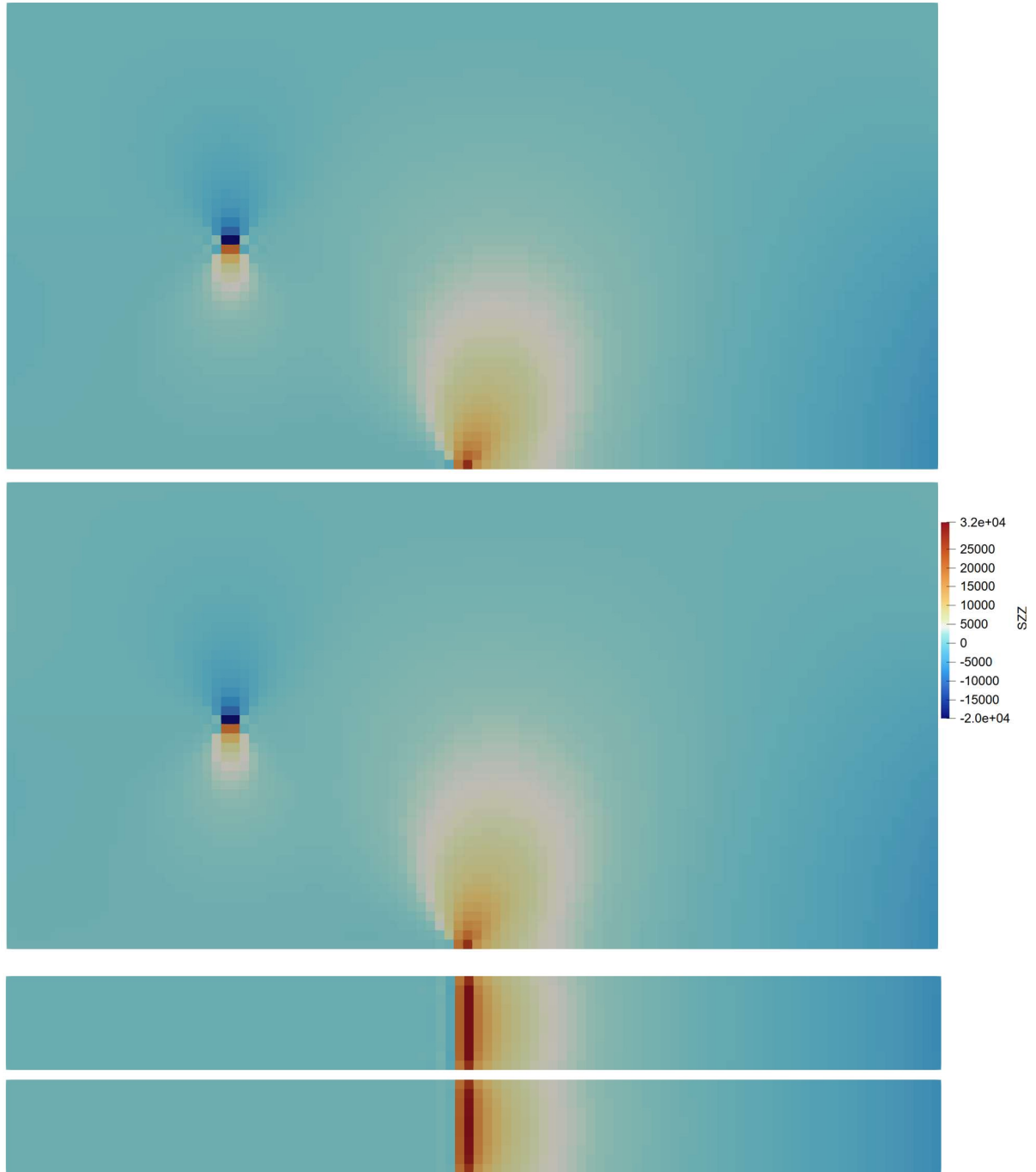


Figure 4: Comparison of vertical stress fields (σ_{33}) in planes (e_2, e_3) and (e_1, e_2) . For each plane the upper field is the FFT-based simulation (using TETRA2 elements) and the lower is the FE simulation (using CAST3M code and linear hexahedral element with full integration).

4.2 : Alternative: Weakly or smoothly applied conditions

When strongly applying kinematic constraints to isolated nodes, or lines of nodes, non-convergence issue for HEX1 elements (see previous section), or very important spurious oscillations for TETRA2 elements (see Figure 5), are reported. Compared to HEX1, TETRA2 elements exhibit very smooth stress

fields and less convergence issue. This section focuses on TETRA2 scheme. To overcome the issue with TETRA2 elements, two alternative methods are proposed:

1. Weakly applied conditions: the displacement is applied to the center of a cube or a square (whether the condition is applied in the volume or at the surface) using an average displacement and reaction forces defined on the same support (8 nodes of the cube or 4 nodes of the square),
2. Smoothly applied conditions: the displacement is applied to a given node, but reaction forces are smoothly distributed on a larger support (27 nodes or 9 nodes whether the condition is applied in the volume or at the surface).

In both cases and consistently with the previous subsection, the modification in Algorithm 1 is limited to the two functions $proj_U$ and $proj_P$.

4.2.1 : Weakly applied conditions

Considering a condition in the volume, instead of applying a displacement to a single node, the displacement is now applied to a voxel center. As the grid of voxel centers are not the support of the discrete displacement field, an interpolation is used from nodes to center, so that instead of the strong condition $\tilde{u}_{j_0}^{i_0} = U_{j_0}^{i_0}$ applied to node i_0 for component j_0 , the condition applied to the center of element i_0 reads:

$$\frac{1}{8} \sum_{i \in V(i_0)} \tilde{u}_{j_0}^i = U_{j_0}^{i_0} \quad \text{with } V(i_0) = 8 \text{ nodes of element } i_0 \quad (10)$$

This condition is a linear relationship between displacement of different nodes. To introduce this condition in Algorithm 1, the current displacement field is corrected in $proj_U$ with:

$$proj_U: \tilde{u}_{j_0}^i = \tilde{u}_{j_0}^i + U_{j_0}^{i_0} - \frac{1}{8} \sum_{k \in V(i_0)} \tilde{u}_{j_0}^k \quad \text{for } i \in V(i_0) \quad (11)$$

When considering the static condition applied strongly, the associated equation consists of forcing the equilibrium with $\text{div}_D(\underline{\sigma})_{j_0}^{i_0} + f_{j_0}^{i_0} = 0$, so that in the algorithm is simply $p_{j_0}^{i_0} = 0$ in $proj_P$ (see section 4.1.1). For the weak condition here, the reaction force $f_{j_0}^{i_0}$ is now distributed on the 8 nodes of the element so that the equilibrium condition on these nodes reads:

$$\text{div}_D(\underline{\sigma})_{j_0}^i + \frac{1}{8} f_{j_0}^{i_0} = 0 \quad \text{for } i \in V(i_0) \quad (12)$$

And, consequently:

$$\text{div}_D(\underline{\sigma})_{j_0}^i - \frac{1}{8} \sum_{i \in V(i_0)} \text{div}_D(\underline{\sigma})_{j_0}^i = 0 \quad \text{for } i \in V(i_0) \quad (13)$$

To introduce this static condition in Algorithm 1, the current field $\mathbf{p}$ must be corrected in $proj_P$ with:

$$proj_P: p_{j_0}^i = p_{j_0}^i - \frac{1}{8} \sum_{k \in V(i_0)} p_{j_0}^k \quad \text{for } i \in V(i_0) \quad (14)$$

The present condition applied in volume to voxel centers, can be straightforwardly transposed to a condition applied at the surface to the center of a voxel face located at the boundary. The only difference is that $V(i_0)$ consists of four nodes (i.e. the corners of the voxel face) instead of eight nodes (i.e. the corners of the voxel).

4.2.2 : Smoothly applied conditions

Another proposition to avoid the oscillations using TETRA2 elements with kinematic conditions on isolated nodes, consists in smoothly redistribute the reaction forces on neighboring nodes.

Considering a kinematic condition applied to a node i_0 , located in the volume, for component j_0 , Algorithm 1 is applied with the same correction as in section 4.1 for a strongly applied condition:

$$proj_U: \tilde{u}_{j_0}^{i_0} = U_{j_0}^{i_0} \quad (15)$$

The difference with a strongly applied condition (section 4.1) is that the reaction force located at node i_0 is now smoothed over the 26 neighboring nodes, i.e. the corners of the 2x2x2 elements cell centered on node i_0 , according to different weights w_{ME} , w_{MF} and w_{Co} , where the subscript ME stands for nodes located at the middle of edges (12 points), MF for nodes located at the middle of faces (6 points), and Co for corners (8 points). To account for reaction redistribution, the reaction $f_{j_0}^{i_0}$ evaluated at point i_0 (first line below) is complemented by additional forces located on the 26 neighboring nodes. Then, equilibrium equations around node i_0 are modified as follows:

$$\begin{aligned} \text{div}_D(\underline{\sigma})_{j_0}^{i_0} + f_{j_0}^{i_0} &= 0 \\ \text{div}_D(\underline{\sigma})_{j_0}^i + w_i f_{j_0}^{i_0} &= 0 \quad \text{for } i \in V'(i_0) = 26 \text{ nodes neighbors of } i_0 \end{aligned} \quad (16)$$

It must be noticed that no additional unknown has been added to $f_{j_0}^{i_0}$ that remains the only unknown associated to the prescribed condition on $\tilde{u}_{j_0}^{i_0}$. The introduction of the above equilibrium equations is done in Algorithm 1 through a correction of the current field $\mathbf{p}$ applied in $proj_P$ with:

$$\begin{aligned} proj_P: f_{j_0}^{i_0} &= -p_{j_0}^{i_0} \\ p_{j_0}^{i_0} &= 0 \quad (= p_{j_0}^{i_0} + f_{j_0}^{i_0}) \\ p_{j_0}^i &= p_{j_0}^i + w_i f_{j_0}^{i_0} \quad \text{for } i \in V'(i_0) = 26 \text{ nodes neighbors of } i_0 \end{aligned} \quad (17)$$

The method has been introduced for a condition applied to a node located in the volume, its modification towards a node located at the surface is straightforward: instead of considering a neighborhood of 26 nodes, only the 8 neighbors located at the surface are considered. Finally, the definition of the weights is given in table below for the two cases. The total reaction force associated to the kinematic condition is then equal to $\left(1 + \frac{12}{4} + \frac{6}{2} + \frac{8}{8}\right) f_{j_0}^{i_0} = 8f_{j_0}^{i_0}$ and $\left(1 + \frac{4}{2} + \frac{4}{4}\right) f_{j_0}^{i_0} = 4f_{j_0}^{i_0}$, respectively for volume and surface condition.

	Volume	Surface
w_{ME}	1/4	1/2
w_{MF}	1/2	×
w_{Co}	1/8	1/4

Table 2: Definition of the weights used to smooth the reaction force for the cases of a node located in the volume (redistribution over 27 nodes) or at the surface (redistribution over 9 nodes). Co, ME, MF, stand for nodes located at Corner, Middle Edge and Middle Face of a 2x2x2 volume elements cell (or a 2x2 surface elements cell).

4.2.3 : Results on a CT-like specimen

First, weakly applied conditions have been used (see Figure 3 - bottom) to overcome the convergence issue observed using HEX1 elements together with strong BCs applied to the complete line of nodes located at (0:10,25,25). The condition is weakly applied to the line of elements with centers located at (0.5:9.5,24.5,24.5) using the same equations (10) to (14), just replacing $V(i_0)$ the set of nodes of element i_0 by V^* the set of 44 nodes belonging to the concerned elements. Convergence is achieved and, in spite of small oscillations, stress field compares nicely to the results obtained with the TETRA2 scheme. However, these spurious oscillations, associated with hourglass phenomenon, are more visible on the displacement field as observed on the deformed configuration.

Secondly, to demonstrate the issue arising with TETRA2 elements when a displacement is applied to a single node, the same configuration as shown in Figure 2 is considered. The only difference is that the load is applied to a single node located at (2,24,24) rather than to the entire line of nodes (0:10,24,24). As observed on Figure 5-right, despite the convergence of the algorithm, the solution is massively affected by artifacts observed on the displacement field. At first sight, this result is quite surprising. However, the explanation can be found in the analysis made by Finel [24] when introducing TETRA2 elements. Actually, if the simplified description proposed in [39] is of practical interest, the original description [24] demonstrates that the problem solved on the complete grid consists of two decoupled problems, defined on two different geometric supports (i.e. the two subgrids of tetrahedra reported on Figure 6), solved simultaneously. As a consequence, for this type of element, applying the loading to a single node will let one of the two problems unloaded. Indeed, when looking at Figure 5-right part, it can be noticed that half of the nodes remains on the undeformed configuration and the other part has a displacement consistent with Figure 5-left part obtained with weakly applied condition to an element centered at (2.5,24.5,24.5).

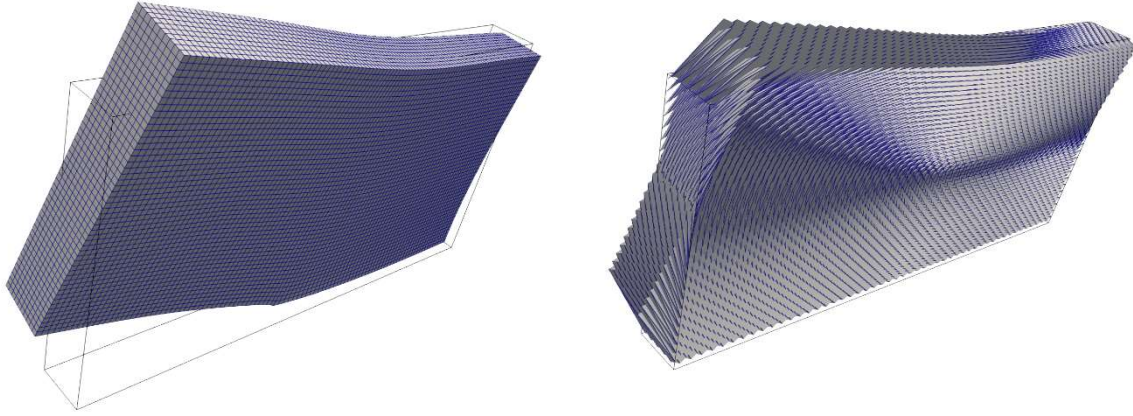


Figure 5: Representation of the deformed configuration of a CT-like specimen submitted to a vertical load on a single point that do not belong to the plane of symmetry so that the specimen opens and twists as expected. On the right, the displacement is applied strongly to a single node (position (2,24,24)) exhibiting important artifacts of the displacement field associated to the TETRA2 elements. On the left, the displacement is applied weakly to an element center (position (2.5,24.5,24.5)) with a complete disappearance of artifacts.

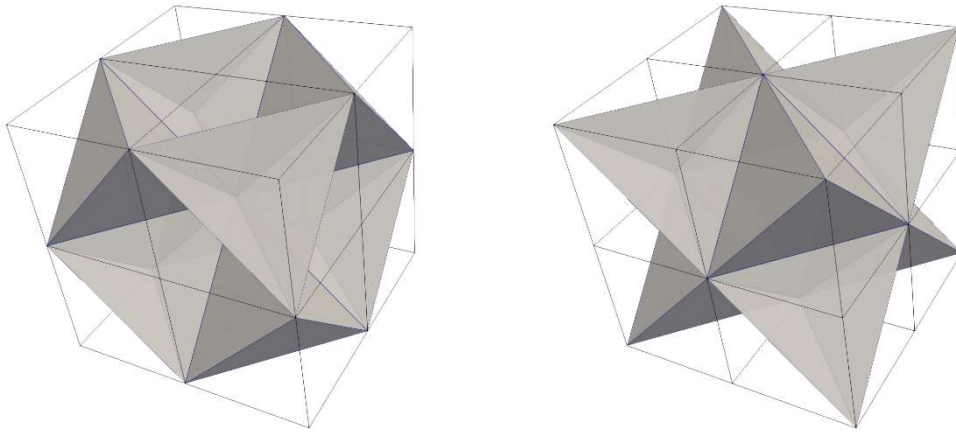


Figure 6 : Representation of the two subgrids of tetrahedra, supports of the two decoupled problems simultaneously solved when considering TETRA2 elements (see [24] for a deeper explanation).

Finally, a simulation with smoothly applied condition with the prescribed displacement applied at node (2,24,24) has been performed. The result is very similar w.r.t. the simulation using weakly applied BCs at the center of element at (2.5,24.5,24.5). A slight discrepancy is observed due to the minor difference of the location where the displacement is applied (a half-voxel difference). Because of the strong similarity with Figure 5-left part, this additional result is not reported in a figure. More interestingly, it must be noticed that the number of iterations at convergence is the same (332) for both simulations.

To conclude, we have proposed two different ways to apply local Dirichlet BCs compatible with the TETRA2 scheme for which applying 'strongly' a displacement to a single node is not relevant.

4.3 : Discussion : minimization under equality constraint

In the previous section, the resolution of the discrete problem was proposed from the perspective of local equations. The purpose of the section is to look at the same problems from the perspective of constrained minimization problems and associated linear systems. This approach is well-known by the FE community and can be found in different handbooks (see for example section 4.1 devoted to Lagrange multipliers in the book of Yastrebrov [44], also used in the next section to deal with contact mechanics).

For strongly applied conditions (see section 4.1), the set of local equations (8) for the discrete problem can be re-formulated as a minimization problem subject to equality constraints as follows:

$$\inf_{[\tilde{u}]} (J([\tilde{u}])) = \inf_{[\tilde{u}]} \left(\frac{1}{2} [\tilde{u}]^T \llbracket K \rrbracket [\tilde{u}] \right) \quad \text{with } [\tilde{u}] \text{ subject to } [\tilde{u}_{j_0}^{I_0}] = [U_{j_0}^{I_0}] \quad (18)$$

Vector $[\tilde{u}]$ gathers the displacements unknowns at all the point that are not imposed to zero at boundary through Anti-Symmetry extension (i.e. Dirichlet condition imposed through the use of DTT). Vector $[U_{j_0}^{I_0}]$ gathers the values of the displacements imposed to $[\tilde{u}_{j_0}^{I_0}]$, a subset of $[\tilde{u}]$ (see section 4.1 for the definition of I_0 and J_0 , gathering respectively the node location and the components subitted to local Dirichlet conditions). Finally, matrix $\llbracket K \rrbracket$ is built from the local discrete operator $\mathbf{div}_D \left(\mathbb{C} : \left(\nabla_D^s(\tilde{\mathbf{u}}) \right) \right)$ so that, for example, the equilibrium condition $\mathbf{div}_D \left(\mathbb{C} : \left(\nabla_D^s(\tilde{\mathbf{u}}) \right) \right) = 0$ for any grid point is equivalent to $\llbracket K \rrbracket [\tilde{u}] = [0]$. Then, the constrained problem (18) can be rewritten using its Lagrangian formulation leading to problem (19), corresponding to the definition of a saddle point (.

$$\sup_{[f_{j_0}^{I_0}]} \inf_{[\tilde{u}]} \left(J([\tilde{u}]) + [f_{j_0}^{I_0}]^T ([\tilde{u}_{j_0}^{I_0}] - [U_{j_0}^{I_0}]) \right) \quad (19)$$

In this formulation, $[\tilde{u}]$ is no more constrained and a vector of Lagrange multipliers $[f_{j_0}^{I_0}]$ (interpreted in section 4.1 as reaction forces) is added to $[\tilde{u}]$ as unknown vector. Note that there is one Lagrange multiplier per relation so that the size of $[f_{j_0}^{I_0}]$ is equal to the size of $[\tilde{u}_{j_0}^{I_0}]$. Finally, the first-order optimality conditions (derivation w.r.t. to $[\tilde{u}]$ and $[f_{j_0}^{I_0}]$) allows to build the following linear system:

$$\begin{bmatrix} \llbracket K \rrbracket & \llbracket A \rrbracket^T \\ \llbracket A \rrbracket & \llbracket 0 \rrbracket \end{bmatrix} \begin{bmatrix} [\tilde{u}] \\ [f_{j_0}^{I_0}] \end{bmatrix} = \begin{bmatrix} [0] \\ [U_{j_0}^{I_0}] \end{bmatrix} \quad (20)$$

The matrix $\llbracket A \rrbracket$ has the dimension (size of $[f_{j_0}^{I_0}]$, size of $[\tilde{u}]$). It ensures the correspondence between the indices of $[\tilde{u}]$ subject to constraints and the corresponding values imposed in vector $[U_{j_0}^{I_0}]$. On the other hand, $\llbracket A \rrbracket^T$ ensure the correspondence between the reaction forces $[f_{j_0}^{I_0}]$ and the indices of $[\tilde{u}]$ subject to constraints. In that case, the matrix $\llbracket A \rrbracket$ has a rather simple form with zeros almost everywhere and a few ones to ensure correspondence. For example, for a single constraint on node i_0 and component j_0 , matrix $\llbracket A \rrbracket$ has a single line and a single “one” value at the position of the unknown $\tilde{u}_{j_0}^{i_0}$ in $[\tilde{u}]$ as shown below.

$$\llbracket A \rrbracket = [0 \dots 010 \dots 0] \quad (21)$$

Adding another constraint of the same type is simply done by adding a new line, of the same type, in matrix $\llbracket A \rrbracket$.

To summarize, this linear system (equation (20)), equivalent to the set of local equations (8), provides the solution of a constrained minimization problem, through the solution of a saddle point problem by introducing Lagrange multiplier. The method is very common and standard in FE codes. The present paper demonstrates the ability of the proposed FFT-based solver to solve this type of problems with simple equality constraints such as the strongly applied conditions (i.e. $(\tilde{\mathbf{u}}^{I_0})_{J_0} = (\mathbf{U}^{I_0})_{J_0}$).

For weakly applied conditions, compared to the previous case, equation (10) now imposes linear relations between kinematic unknowns. The same approach as before can be used, associating a Lagrange multiplier to any relation. Matrix $\llbracket A \rrbracket$ now stores the linear relations corresponding to equation (10) and, for a single constraint on element i_0 and component j_0 , has the form:

$$\llbracket A \rrbracket = [0. \frac{1}{8} 0. 0. \frac{1}{8} 0. 0. \frac{1}{8} 0. 0. \frac{1}{8} 0. 0. \frac{1}{8} 0. 0. \frac{1}{8} 0. 0. \frac{1}{8} 0.] \quad (22)$$

The eight values $\frac{1}{8}$ are located at positions of $\tilde{u}_{j_0}^i$ in $[\tilde{\mathbf{u}}]$ (for the eight nodes i , corners of element i_0). Regarding equation (20), matrix $\llbracket A \rrbracket^T$ will dispatch the reaction force $f_{j_0}^{i_0}$ on the eight nodes i , corners of element i_0 , as done in the local equations (12). Therefore, the present FFT-based solver demonstrates its ability to solve minimization problems with linear equality constraints. The application in section 4.2.1 is an example of this possibility, but the same approach can be followed to apply any other kinematic constraints.

Finally, for smoothly applied conditions (see section 4.2.2), the strong kinematic condition corresponds to matrix $\llbracket A \rrbracket$ in equation (23) and the redistribution of the reaction forces associated to equation (16) corresponds to matrix $\llbracket B \rrbracket$. This problem can be regarded as a minimization problem introducing the concept of “diffuse” Lagrange multipliers, an originality to the author knowledge, that is not reported in standard FE codes but could be introduced as well.

$$\begin{bmatrix} \llbracket K \rrbracket & \llbracket B \rrbracket \\ \llbracket A \rrbracket & \llbracket 0 \rrbracket \end{bmatrix} \begin{bmatrix} [\tilde{\mathbf{u}}] \\ [f_{I_0}^{J_0}] \end{bmatrix} = \begin{bmatrix} [0] \\ [U_{I_0}^{J_0}] \end{bmatrix} \quad (23)$$

As the proposed FFT-based solver has the ability to solve minimization problems subject to equality constraints, the next section focuses on a further extension towards inequality constraints as observed in unilateral contact mechanics.

5 : Contact mechanics – application to spherical indentation

In this section, the FFT-based solver proposed in Algorithm 1 to account for equality constraints is modified to account for unilateral constraints associated to rigid and frictionless contact mechanics. A homogeneous cubic volume of size L^3 is considered with the face S_1^0 submitted to null-Dirichlet BCs, null-Neumann BCs on the four faces S_J^α ($\alpha = 0,1$ and $J = 2,3$), and contact conditions on face S_1^1 (see definition of S_J^α in section 3.2.1). The rigid indenter is a sphere $\mathcal{S}$ of radius R_s and center $\mathbf{O}_s$ initially located at position $[L + R, 0.5L, 0.5L]$. The loading is given by the displacement of the sphere $\mathbf{U}_S =$

$U_S \mathbf{e}_1$. The contact conditions on surface S_1^1 are associated with the existence of a contact zone $\mathcal{C}$, defined on the deformed configuration, through the Karush-Kuhn-Tucker (KKT) conditions with frictionless assumption. The contact problem is written as follows:

$$\begin{cases} \underline{\sigma} \cdot \mathbf{n} = \mathbf{0} & \text{on } S_1^1/\mathcal{C} \\ g > 0 & \text{on } S_1^1/\mathcal{C} \\ \mathbf{n}_c \cdot \underline{\sigma} \cdot \mathbf{n}_c < 0 & \text{on } \mathcal{C} \\ g = 0 & \text{on } \mathcal{C} \\ \underline{\sigma} \cdot \mathbf{n}_c - (\mathbf{n}_c \cdot \underline{\sigma} \cdot \mathbf{n}_c) \mathbf{n}_c = \mathbf{0} & \text{on } \mathcal{C} \end{cases} \quad (24)$$

In this set of contact conditions, the outer normal is $\mathbf{n}$. For any point M' of the surface S_1^1 in the deformed configuration, M'_s is the radial projection of M' on the sphere located at $\mathbf{O}'_s$ (position of the sphere center), and the potential contact normal is defined by $\mathbf{n}_c = -\mathbf{O}'_s M' / \|\mathbf{O}'_s M'\|$. The gap is then defined as $g = (\mathbf{O}'_s M'_s - \mathbf{O}'_s M') \cdot \mathbf{n}_c$. Hence, out of the contact zone, the surface is free (1st equation in problem (24)) and the gap is positive (2nd equation in problem (24)). In the contact zone, the gap is null (4th equation in problem (24)), the normal traction vector is negative (3rd equation in problem (24)) and the tangential traction vector is null (5th equation in problem (24)) because of frictionless assumption.

Following the previous section, the introduction of the FFT-based solver is proposed from local equations, in the small and finite strains setting, and, after an analysis of the application results, the viewpoint of minimization problem under inequality constraint is adopted.

5.1 : Small strain implementation

After regular discretization of the VE, the discrete problem is solved using the active set strategy (see for instance the handbook of Yastrebov about numerical methods in contact mechanics [44]) to determine the contact zone. Starting with an initial active contact zone $\mathcal{C}$ (i.e. active set) defined by the set of discrete points violating the gap condition after a displacement increment of the sphere, the algorithm consists in applying iteratively the following two steps:

1. Solve the problem with the BCs:

$$\begin{cases} \underline{\sigma} \cdot \mathbf{e}_1 = \mathbf{0} & \text{on } S_1^1/\mathcal{C} \\ g = 0 & \text{on } \mathcal{C} \\ \underline{\sigma} \cdot \mathbf{n}_c - (\mathbf{n}_c \cdot \underline{\sigma} \cdot \mathbf{n}_c) \mathbf{n}_c = \mathbf{0} & \text{on } \mathcal{C} \end{cases} \quad (25)$$

2. Update the active contact zone $\mathcal{C}$ as follows:

$$\begin{cases} \text{for } M \in S_1^1/\mathcal{C} & : & \text{if } (g(M) < 0) & M \in \mathcal{C} \\ \text{for } M \in \mathcal{C} & : & \text{if } ((\mathbf{n}_c \cdot \underline{\sigma} \cdot \mathbf{n}_c)(M) > 0) & M \notin \mathcal{C} \end{cases} \quad (26)$$

The two steps are detailed below and then incorporated in the accelerated fixed-point FFT-based solver proposed in the previous section.

5.1.1: Step 1

After spatial discretization, the resolution of step 1 is done using reaction forces (i.e. Lagrange multipliers) as done in problem (8). The scalar $f_{n_c}^{\mathcal{C}}$ are the values of the reaction forces oriented by the

vector $\mathbf{n}_c$ for all the points of $\mathcal{C}$. The kinematic condition (fourth equation in problem below) imposes that any point of $\mathcal{C}$ must be located at the surface of the sphere in the deformed configuration.

$$\begin{cases} \mathbf{div}_D(\underline{\sigma}) + f_{n_c}^c \mathbf{n}_c = 0 & \text{in } \Omega^\infty \\ \underline{\varepsilon} = \underline{\nabla}_D^s(\tilde{\mathbf{u}}) & \text{in } \Omega^\infty \\ \underline{\sigma} = \mathbb{C} : \underline{\varepsilon} & \text{in } \Omega \\ \tilde{\mathbf{u}}(M) = \mathbf{M}\mathbf{O}'_s + R_s \mathbf{n}_c & \text{in } \mathcal{C} \\ \tilde{\mathbf{u}} \text{ appropriate symmetries} & \text{in } \Omega^\infty \\ \underline{\sigma} \text{ appropriate symmetries} & \text{in } \Omega^\infty \end{cases} \quad (27)$$

In the present case, the appropriate symmetries are associated with null-Dirichlet on face S_1^0 and null-Neumann on the other faces, hence all the components of $\tilde{\mathbf{u}}$ have the symmetries A on face S_1^0 and S on the five other faces. The symmetries of $\underline{\sigma}$, not reported here, are consistent with Table 1. Note that the condition $\underline{\sigma} \cdot \mathbf{e}_1 = \mathbf{0}$ on $S_1^1/\mathcal{C}$ is then satisfied by this choice of symmetries.

The resolution can be done as in section 4, with a fixed-point algorithm corresponding to the succession of equations given in problem (28), omitting convergence acceleration for the sake of clarity.

$$\begin{cases} proj_U : \tilde{\mathbf{u}}(M) = \mathbf{M}\mathbf{O}'_s + R_s \mathbf{n}_c & \forall M \in \mathcal{C} \\ \underline{\sigma} = \mathbb{C} : \underline{\nabla}_D^s(\tilde{\mathbf{u}}) \\ \mathbf{p} = \mathbf{div}_D(\underline{\sigma}) \\ proj_P : (\mathbf{p} \cdot \mathbf{n}_c)(M) = 0 & \forall M \in \mathcal{C} \\ \mathbf{p} = \mathbf{p} - \mathbf{div}_D \left(\mathbb{R}_0 : \underline{\nabla}_D(\tilde{\mathbf{u}}) \right) \\ \hat{\tilde{\mathbf{u}}} = \hat{\mathbb{G}}_D(\hat{\mathbf{p}}) \end{cases} \quad (28)$$

As in section 4, the local Dirichlet conditions are imposed through projections $proj_U$ and $proj_P$. On the one hand, $proj_U$ modifies the current field $\tilde{\mathbf{u}}$, so that the points of $\mathcal{C}$ in the deformed configuration are located on the sphere. On the other hand, $proj_P$ vanishes $\mathbf{p} \cdot \mathbf{n}_c$ on $\mathcal{C}$ so that systematically $\mathbf{div}_D(\underline{\sigma}) \cdot \mathbf{n}_c + f_{n_c}^c = 0$, with $f_{n_c}^c$ the normal reaction force to be evaluated as a post-treatment once achieved the convergence of the algorithm.

5.1.2: Step 2

The first equation in problem (26) consists in evaluating the gap $g(M) = (\mathbf{O}'_s \mathbf{M}'_s - \mathbf{O}'_s \mathbf{M}') \cdot \mathbf{n}_c(M)$ (with $\mathbf{n}_c(M) = -\mathbf{O}'_s \mathbf{M}' / \|\mathbf{O}'_s \mathbf{M}'\|$) for any point of the surface $S_1^1/\mathcal{C}$. If the gap is negative, the point M is added to $\mathcal{C}$.

The second equation in problem (26) is replaced by a condition on the normal reaction forces $f_{n_c}^c(M)$ (i.e. Lagrange multipliers) evaluated for any point M in $\mathcal{C}$. If the reaction force $f_{n_c}^c(M)$ is positive, the point is removed from $\mathcal{C}$.

5.1.3: FFT-based algorithm

In practice, the two iterative algorithms (active set strategy and accelerated fixed-point algorithm) are gathered in Algorithm 2, an accelerated fixed-point algorithm with a conditional update of the contact

zone $\mathcal{C}$. To account for the non-linear nature of the problem, the displacement of the indenter is increased incrementally.

1. Initial $\tilde{\mathbf{u}} = \tilde{\mathbf{u}}$ of previous increment
2. Increase increment loading $\rightarrow O'_s$
3. Initialize active contact zone $\rightarrow \mathcal{C}$
4. $proj_U : \tilde{\mathbf{u}}(M) = \mathbf{M}O'_s + R_s \mathbf{n}_c(M) \quad \forall M \in \mathcal{C}$
5. Loop $i \geq 0$
6. if (ACV_U)
7. if ($i > 0$) $ACV_{storeR}(i, \tilde{\mathbf{u}})$
8. if ($i > 0$ & modulo(i, mod_{ACV}) = 0) $ACV_{accelerate} \rightarrow \tilde{\mathbf{u}}$
9. $ACV_{storeS}(i, \tilde{\mathbf{u}})$
10. $\underline{\sigma} = \mathbb{C} : \nabla_D^s(\tilde{\mathbf{u}})$
11. $\mathbf{p} = \text{div}_D(\underline{\sigma})$
12. if equilibrium($\mathbf{p}$): EXIT Loop
13. $proj_P : \mathbf{p}(M) = \mathbf{p}(M) - ((\mathbf{p} \cdot \mathbf{n}_c) \mathbf{n}_c)(M) \quad \forall M \in \mathcal{C}$
14. $\text{eval}(\mathcal{V}_{gap}^i, \mathcal{V}_{react}^i)$
15. if ($\{\mathcal{V}_{gap}^i, \mathcal{V}_{react}^i\} = \{\mathcal{V}_{gap}^{i-1}, \mathcal{V}_{react}^{i-1}\}$)
16. $\mathcal{C}^{old} = \mathcal{C}$
17. update $\mathcal{C}$
18. if ($\mathcal{C} \neq \mathcal{C}^{old}$) $i = 0$ (to reinitialize ACV arrays)
19. $\mathbf{p} = \mathbf{p} - \text{div}_D(\mathbb{R}_0 : \nabla_D(\tilde{\mathbf{u}}))$
20. if (ACV_P)
21. if ($i > 0$) $ACV_{storeR}(i, \tilde{\mathbf{p}})$
22. if ($i > 0$ & modulo(i, mod_{ACV}) = 0) $ACV_{accelerate} \rightarrow \tilde{\mathbf{p}}$
23. $ACV_{storeS}(i, \tilde{\mathbf{p}})$
24. $DT(\mathbf{p}) \rightarrow \hat{\mathbf{p}}$
25. $\hat{\tilde{\mathbf{u}}} = \hat{\mathbb{G}}_D(\hat{\mathbf{p}})$
26. $iDT(\hat{\tilde{\mathbf{u}}}) \rightarrow \tilde{\mathbf{u}}$
27. $proj_U : \tilde{\mathbf{u}}(M) = \mathbf{M}O'_s + R_s \mathbf{n}_c(M) \quad \forall M \in \mathcal{C}$

Algorithm 2 : Description of the FFT-based algorithm proposed for spherical indentation (for an increment of loading) using a small strain framework. Compared to Algorithm 1, the main differences are highlighted in green for the update of the contact zone, and in red for the functions $proj_U$ and $proj_P$, specialized for the indentation application.

The goal of the algorithm is to find the solution $\tilde{\mathbf{u}}$ after an incremental displacement of the indenter. The initial guess for $\tilde{\mathbf{u}}$ is the field at the end of previous increment and the initial contact zone $\mathcal{C}$ is defined as the set of points violating the gap condition (i.e. $g(M) < 0$) after the incremental displacement of the sphere.

The accelerated fixed-point algorithm is very close to Algorithm 1, with a specialization of the functions $proj_U$ and $proj_P$ (red lines) to apply the Dirichlet constraints in the contact zone $\mathcal{C}$ as explained in section 5.1.1, and a conditional update of the contact zone (green lines). For that purpose, at each iteration i , the set of points violating the gap condition $\mathcal{V}_{gap}^i$ (first equation in problem (26)) is evaluated as well as the set of points violating the normal stress condition $\mathcal{V}_{react}^i$ (second equation in problem (26)). Instead of using $(\mathbf{n}_c \cdot \underline{\sigma} \cdot \mathbf{n}_c) > 0$, the condition is applied to the normal reaction forces,

$f_{n_c}^c > 0$, with $f_{n_c}^c = -\mathbf{div}_D(\underline{\sigma}) \cdot \mathbf{n}_c$, evaluated on the points of $\mathcal{C}$ (i.e. a subset of face S_1^1) using the discrete derivation of $\underline{\sigma}$ considering an additional layer of null stress on the external side of S_1^1 . Before updating the contact zone $\mathcal{C}$, the solution field must be precise enough, but it is useless to iterate until a very precise solution as soon as the contact zone is not correct. Hence, it is proposed that the contact zone is updated if the sets of points $\mathcal{V}_{gap}^i$ and $\mathcal{V}_{react}^i$ are both identical to the sets of points evaluated at the previous iteration. In other terms, the contact zone is updated if the sets of points candidates for the update are stable from one iteration to another. Note that an additional condition on the equilibrium condition (with a higher tolerance than the one used for the exit condition) is also required to ensure a sufficient precision before update (a value of 10^{-2} is used compared to the standard 10^{-4} tolerance). Importantly, concerning convergence acceleration, the iteration indicator i is reset to 0 when the contact zone is modified (line 18 in Algorithm 2) so that convergence acceleration is restarted (otherwise the arrays storing residual and solution fields would mix fields obtained for two different contact zones, or in other words, for two different problems).

5.2 : Finite strain implementation

The SS implementation proposed above combines equations that do not distinguish initial and deformed configuration and contact conditions (in the contact zone $\mathcal{C}$) applied in the deformed configuration. For a more rigorous treatment, a FS implementation is proposed.

To solve the contact problem with a fixed contact zone $\mathcal{C}$ in step 1 (see section 5.1.1), the set of equations gathered in problem (27) can be reformulated in the finite strain setting using the first Piola-Kirchoff (or Boussinesq), non-symmetric, second-order stress tensor $\underline{\Pi}$:

$$\begin{cases} \mathbf{div}_D(\underline{\Pi}) + f_{n_c}^c \mathbf{n}_c = 0 & \text{in } \Omega^\infty \\ \underline{\tilde{F}} = \underline{1} + \nabla_D(\underline{\tilde{u}}) & \text{in } \Omega^\infty \\ \underline{\Pi} = \mathcal{F}(\underline{\tilde{F}}) & \text{in } \Omega \\ \underline{\tilde{u}}(M) = \mathbf{M}\mathbf{O}'_s + R_s \mathbf{n}_c & \text{in } \mathcal{C} \\ \underline{\tilde{u}} \text{ appropriate symmetries} & \text{in } \Omega^\infty \\ \underline{\Pi} \text{ appropriate symmetries} & \text{in } \Omega^\infty \end{cases} \quad (29)$$

In that case, the precise form of the “behavior” law $\underline{\Pi} = \mathcal{F}(\underline{\tilde{F}})$ is intentionally let general (a simple example can be $\underline{S} = \mathbb{C} : \underline{E}$, with $\underline{\Pi} = \underline{\tilde{F}} \cdot \underline{S}$ and $\underline{S}$ the second Piola-Kirchoff tensor, and $\underline{E} = \frac{1}{2}(\underline{\tilde{F}}^T \underline{\tilde{F}} - \underline{1})$, the Green-Lagrange strain tensor for an elastic material).

To update the contact zone in step 2, the contact conditions on the signs of both the gap and the reaction are exactly the same as in section 5.1.2. In the SS implementation, the reaction $f_{n_c}^c = -\mathbf{div}_D(\underline{\sigma}) \cdot \mathbf{n}_c$ is evaluated on the points of $\mathcal{C}$ taking into account an additional layer of null stress on the external side of S_1^1 . In the FS implementation, the same method is used to evaluate $f_{n_c}^c$, simply replacing $\underline{\sigma}$ by $\underline{\Pi}$ so that $f_{n_c}^c = -\mathbf{div}_D(\underline{\Pi}) \cdot \mathbf{n}_c$.

As the two steps of the algorithm are very similar between small and finite strain frameworks, the FFT-based algorithm implemented for SS (see Algorithm 2) is only slightly modified to account for FS (see Algorithm 3).

1. Initial $\tilde{\mathbf{u}} = \tilde{\mathbf{u}}$ of previous increment
2. Increase increment loading $\rightarrow O'_s$
3. Initialize active contact zone $\rightarrow \mathcal{C}$
4. $proj_U : \tilde{\mathbf{u}}(M) = \mathbf{M}O'_s + R_s \mathbf{n}_c(M) \quad \forall M \in \mathcal{C}$
5. Loop $i \geq 0$
6. if (ACV_U)
7. if ($i > 0$) $ACV_{storeR}(i, \tilde{\mathbf{u}})$
8. if ($i > 0$ & modulo(i, mod_{ACV}) = 0) $ACV_{accelerate} \rightarrow \tilde{\mathbf{u}}$
9. $ACV_{storeS}(i, \tilde{\mathbf{u}})$
10. $\underline{\Pi} = \mathcal{F}(\underline{\mathbf{1}} + \underline{\nabla}_D(\tilde{\mathbf{u}}))$
11. $\mathbf{p} = \mathbf{div}_D(\underline{\Pi})$
12. if equilibrium($\mathbf{p}$): EXIT Loop
13. $proj_P : \mathbf{p}(M) = \mathbf{p}(M) - ((\mathbf{p} \cdot \mathbf{n}_c) \mathbf{n}_c)(M) \quad \forall M \in \mathcal{C}$
14. eval($\mathcal{V}_{gap}^i, \mathcal{V}_{react}^i$)
15. if ($\{\mathcal{V}_{gap}^i, \mathcal{V}_{react}^i\} = \{\mathcal{V}_{gap}^{i-1}, \mathcal{V}_{react}^{i-1}\}$)
16. $\mathcal{C}^{old} = \mathcal{C}$
17. update $\mathcal{C}$
18. if ($\mathcal{C} \neq \mathcal{C}^{old}$) $i = 0$ (to reinitialize ACV arrays)
19. $\mathbf{p} = \mathbf{p} - \mathbf{div}_D(\mathbb{R}_0 : \underline{\nabla}_D(\tilde{\mathbf{u}}))$
20. if (ACV_P)
21. if ($i > 0$) $ACV_{storeR}(i, \tilde{\mathbf{p}})$
22. if ($i > 0$ & modulo(i, mod_{ACV}) = 0) $ACV_{accelerate} \rightarrow \tilde{\mathbf{p}}$
23. $ACV_{storeS}(i, \tilde{\mathbf{p}})$
24. $DT(\mathbf{p}) \rightarrow \hat{\mathbf{p}}$
25. $\hat{\tilde{\mathbf{u}}} = \hat{\mathbb{G}}_D(\hat{\mathbf{p}})$
26. $iDT(\hat{\tilde{\mathbf{u}}}) \rightarrow \tilde{\mathbf{u}}$
27. $proj_U : \tilde{\mathbf{u}}(M) = \mathbf{M}O'_s + R_s \mathbf{n}_c(M) \quad \forall M \in \mathcal{C}$

Algorithm 3 : Description of the FFT-based algorithm proposed for spherical indentation (for an increment of loading) using a Finite strain framework. Compared to the small strain framework, the differences with Algorithm 2 are very limited.

5.4 : Application

The example treated in this section consists of simulating the indentation of a cube with a spherical indenter. The spherical indenter is centered with respect to the contact face. The sphere diameter is equal to the cube edge length of 1mm and the applied displacement indenter is δ . The behavior law is assumed to be elastic isotropic with the Lamé coefficients of steel ($\lambda = 120$ GPa, $\mu = 80$ GPa). For SS assumption, the behavior law is given by ($\underline{\sigma} = \lambda tr(\underline{\sigma}) \underline{\mathbf{1}} + 2\mu \underline{\varepsilon}$) and for FS, the same relation is used replacing the Cauchy stress $\underline{\sigma}$ by the second Piola-Kirchoff stress tensor $\underline{S}$ and the linearized strain $\underline{\varepsilon}$ by the Green-Lagrange strain $\underline{E}$.

For the sake of validation, results are compared to the results of the Hertz theory regarding the reaction force F_{Hertz} as a function of the indenter displacement δ :

$$F_{Hertz} = \frac{4E}{3(1-\nu^2)} \sqrt{R\delta^3} \quad (30)$$

With E and ν the elastic Young modulus and Poisson ratio and R the sphere radius. The validity of Hertz theory being limited to small δ/R ratio (with $R = 0.5\text{mm}$), the simulation covers ratios below 2% ($\delta_1 = 0.01\text{mm}$) for a validation purpose, and up to 20% ($\delta_{max} = 0.1\text{mm}$) to compare the difference between small and finite strain simulations. A reference setup is chosen with a spatial resolution of 65^3 voxels and 80 loading steps. Higher resolutions and loading steps are used below for sensitivity analysis.

Simulations with the reference setup are run using the $\mathbb{R}_0$ tensor proposed by Paux [34] (i.e. $\mathbb{R}_0: \nabla \underline{u} = \lambda_0 \nabla \underline{u} \odot \underline{I} + 2\mu_0 \nabla \underline{u}$, see section 3.2.3) with Lamé coefficients (λ_0, μ_0) proportional to the material Lamé coefficients (λ, μ) . Before going further, the convergence is briefly studied as a function of the preconditioner $\mathbb{R}_0$ to find an approximate optimal choice, i.e. the reference parameters (λ_0, μ_0) . For that purpose, the total number of iterations (summing over the 80 steps) is reported in Table 3. For both FS and SS simulations, an optimal value is found around a factor of 5 (i.e. the reference parameters $(\lambda_0, \mu_0) = 5x(\lambda, \mu)$). This value is kept for SS simulations and, for FS simulations, due to the non-convergence observed for lower factors, a higher value of 10 is used. It can be noticed that, on average, the number of iterations per step is between 92 and 45.

	$\times 1$	$\times 2$	$\times 5$	$\times 10$	$\times 20$
Small Strain	5442	4089	3614	4184	5253
Finite Strain	No Conv.	No Conv.	4863	5354	7413

Table 3 : Total number of iterations using 80 loading steps and a resolution of 65^3 . The factor multiplies the elastic behaviour of the material to define the Lamé coefficients of the preconditioner $\mathbb{C}_0$ (i.e. reference material). No convergence is declared when the number of iterations in a single step reaches 2000.

Taking advantage of the given BCs, to evaluate the reaction force in the FS framework, we simply use $F = A_0 \underline{e}_1 \cdot \langle \underline{\Pi} \rangle \cdot \underline{e}_1$, where A_0 is the area of face S_1^0 (and S_1^1) in the initial configuration and $\langle \underline{\Pi} \rangle$ is the volume average of the Piola-Kirchoff stress tensor over the VE. In the SS framework, we use $F = A_0 \underline{e}_1 \cdot \langle \underline{\sigma} \rangle \cdot \underline{e}_1$, replacing the stress tensor.

Figure 7 and Figure 8 draw the evolution of the force as a function of the indentation depth for a given spatial resolution of 65^3 and different loading steps (20, 40, 80 and 160). Figure 7 presents SS simulation results and FS results are displayed on Figure 8. First, the robustness of the method is emphasized when comparing various loading steps: the coincidence of results demonstrates that, in that range of loading steps, the simulation results are independent of this choice, for both SS and FS cases. Second, the comparison between the Hertz theory and SS simulations is made for small δ/R ratios that corresponds to validity domain of the Hertz theory (see zoom part in Figure 7, with δ below 0.01mm corresponding to $\delta/R = 2\%$). The very good agreement validates both the method and its implementation. The same conclusion can be drawn from the zoom part in Figure 8, validating also the FS case, at least in the range of small δ/R ratios. For larger ratios, up to 20%, it can be noticed that the agreement is still quite good for the SS case. However, the difference with the FS case increases significantly with δ/R , demonstrating the importance of considering FS in that case. Regarding the cumulated number of iterations in Figure 9, it is noticeable that it increases with the number of loading steps, in a similar way for both the SS and FS cases. To understand this, it must be highlighted that, from one step to another, the loading is not proportional as the contact zone increases. Hence, the initialization of the iterative algorithm (line 1 in Algorithm 2 and Algorithm 3) do not consider the results of the previous steps (such as done classically with a linear extrapolation in standard FFT-based solvers with proportional loadings). However, the mean number of iterations per step decreases with

the step size (35, 45, 57 and 65 iterations for 160, 80, 40 and 20 loading steps, in the SS case, and 53, 67, 89, 128 in the FS case). Proposing a better initialization could be an interesting future prospect to reduce the computation cost. As a last comment, for a given number of loading steps, the number of iterations is higher for a FS simulation by a factor of approximately 1.5.

After modifying the loading step for a given resolution in the previous paragraph, Figure 10 and Figure 11 examine the spatial resolution sensitivity for a given number of loading steps (80). A bit surprisingly, for the given range of spatial resolutions (from 33^3 to 129^3) the comparison exhibits a very small resolution sensitivity of the Force-Indentation depth curves, whether for SS or FS cases, for large and small depth (insets in the figures). Regarding the cumulated number of iterations in Figure 12, it is noticeable that it increases with the spatial resolution, in a similar way for both the SS and FS cases. A part of the explanation comes with the number of times the contact zone needs to be updated during the steps. For resolutions of 33, 65 and 129, these numbers are respectively 35, 94 and 164 (for SS simulations). Actually, the higher the number of elements in the contact zone, the higher the number of readjustments of the contact zone is expected. However, these numbers do not solely explain the gaps observed Figure 12 between curves for resolution 33, 65 and 129. A deeper understanding of these gaps is still under investigation.

As a final result, Figure 13 displays the unit-cell in its deformed configuration at the end of the loading, for both SS and FS simulations. The surface of the indenter in its final position is also represented. The deformed shape is qualitatively consistent with expectations: the displacement is smooth without any oscillation; the surface of the indenter coincides with the deformed shape in the contact zone and there is no sign of adhesion with the indenter in the neighborhood of the contact zone. The difference between the SS and FS cases, existing on the macroscopic curve (reaction force-indentation depth) when the δ/R ratio increases (see for example the comparison between Figure 7 and Figure 8), is also observed on the vertical displacement, on Figure 13 for $\delta/R=20\%$ (i.e. last loading step), whose displacement iso-contours are more flat for the FS case.

To summarize, the comparison with Hertz theory for small δ/R ratios validates the new FFT-based solvers proposed in Algorithm 2 and Algorithm 3 to account for spherical indentation and unilateral contact mechanics, respectively for SS and FS cases. For higher ratios, SS and FS results depart from each other, demonstrating the need to account for the non-approximated equations (i.e. FS framework instead of SS hypothesis). The robustness of the method is demonstrated through spatial resolution and loading step sensitivities: the macroscopic curve is very stable around the setup used as reference (65^3 resolution and 80 loading steps). Finally, it is observed that the number of iterations increases with both the spatial resolution and the number of loading steps. A part of this increase is consistent with the algorithms (especially their initializations) and a future prospect will be to reduce it. However, in the present case, the reference setup provides already very stable results and increasing the resolution or the number of loading steps seems useless.

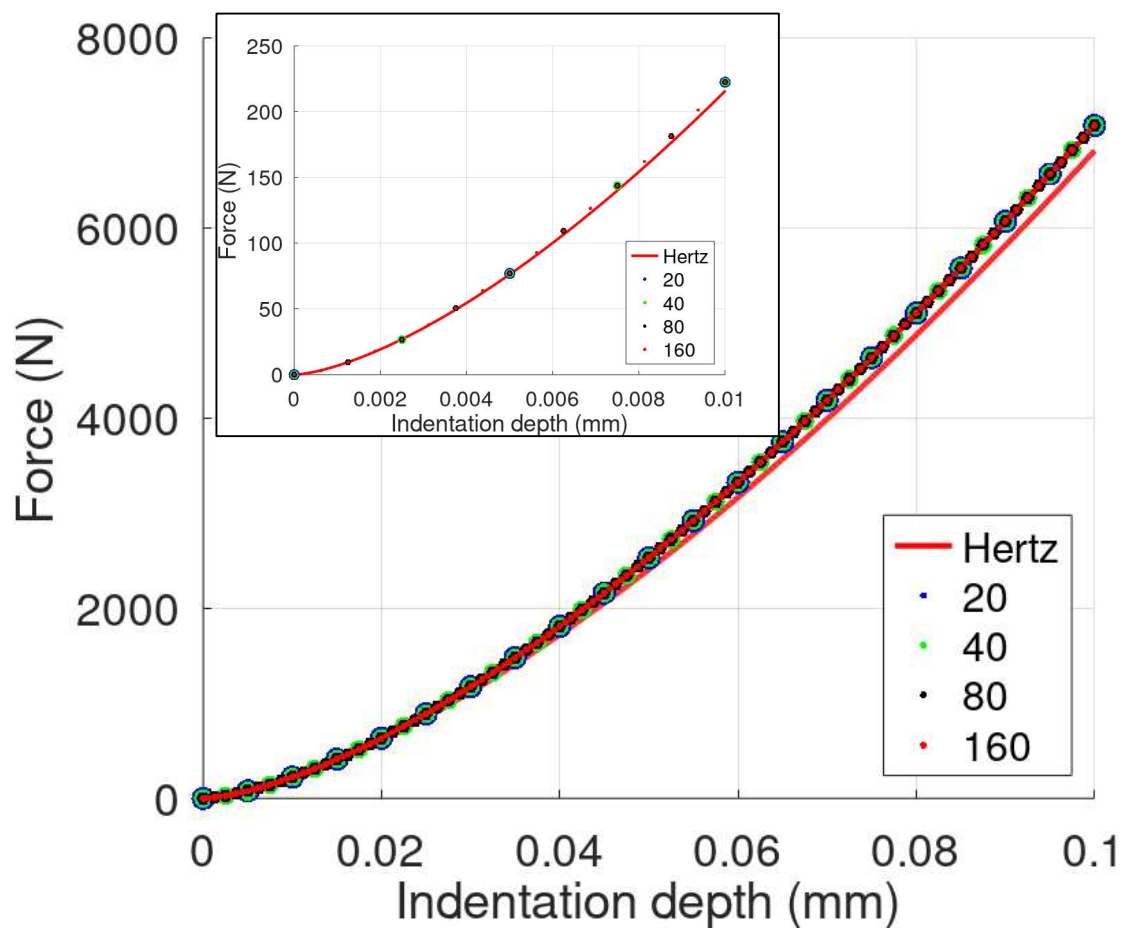


Figure 7 : Force-indentation depth curves from Small Strains simulations with a spatial resolution of 65^3 and 20, 40, 80 and 160 loading steps. The red continuous line represents the curve obtained with the Hertz theory.

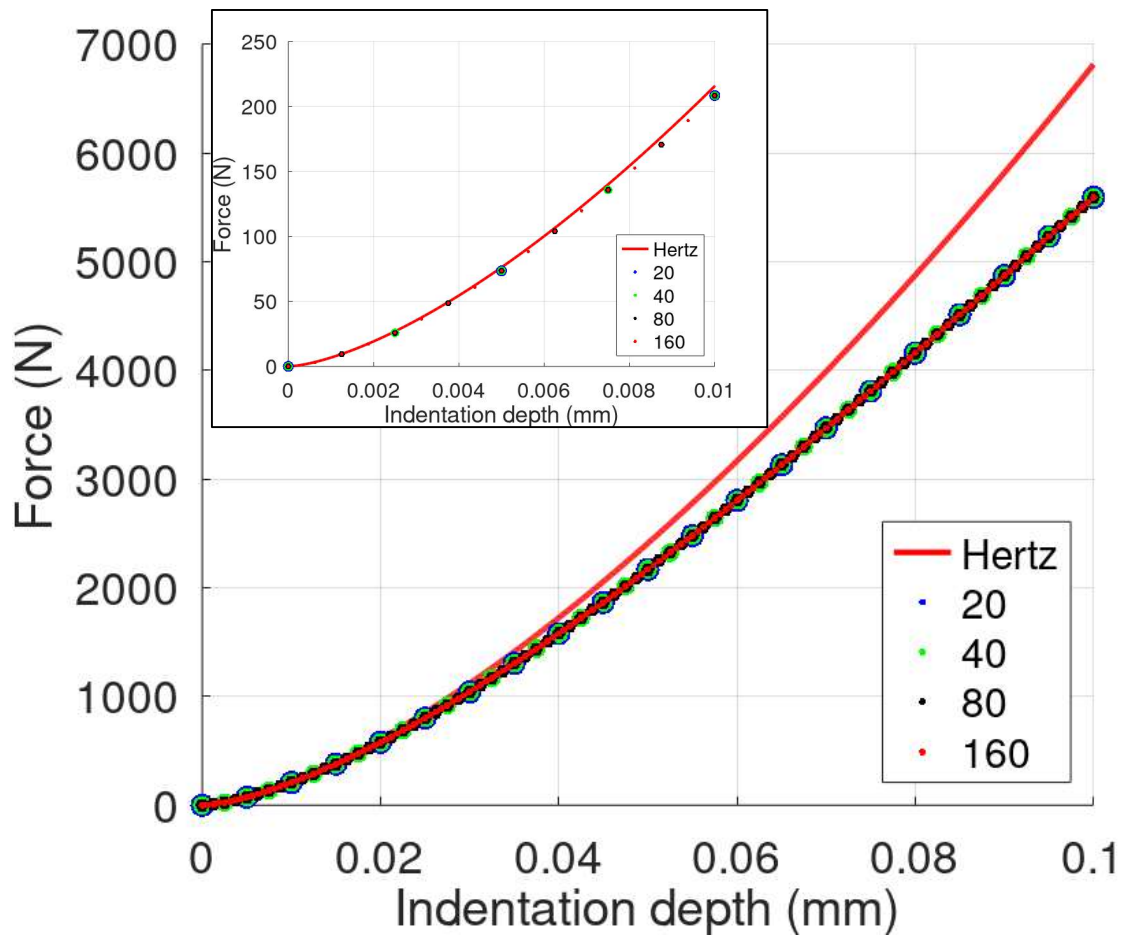


Figure 8 : Force-indentation depth curves from Finite Strains simulations with a spatial resolution of 65^3 and 20, 40, 80 and 160 loading steps. The red continuous line represents the curve obtained with the Hertz theory.

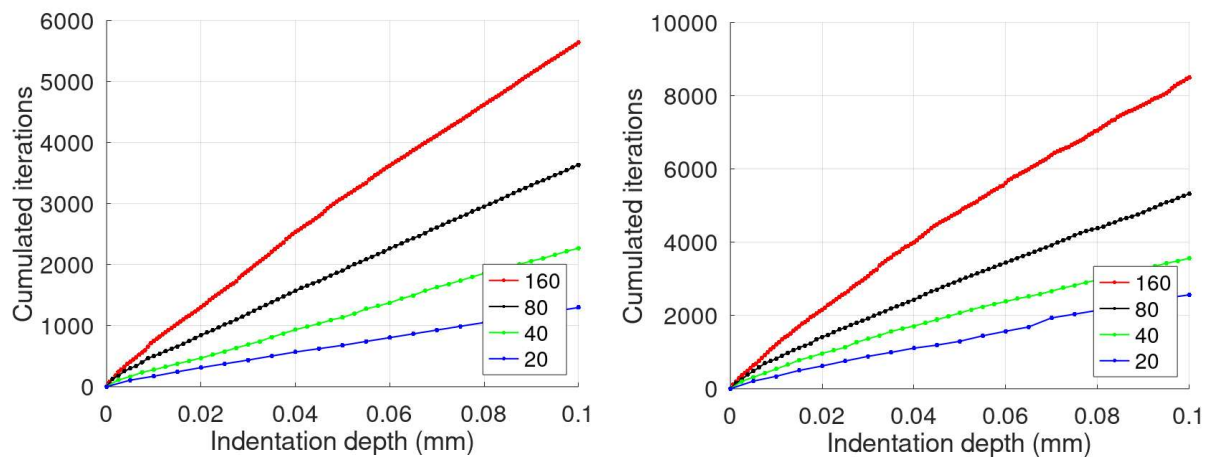


Figure 9 : Cumulated number of iterations for simulations with 20, 40, 80 and 160 loading steps and a spatial resolution of 65^3 : Small Strain case (left) and Finite Strain case (right).

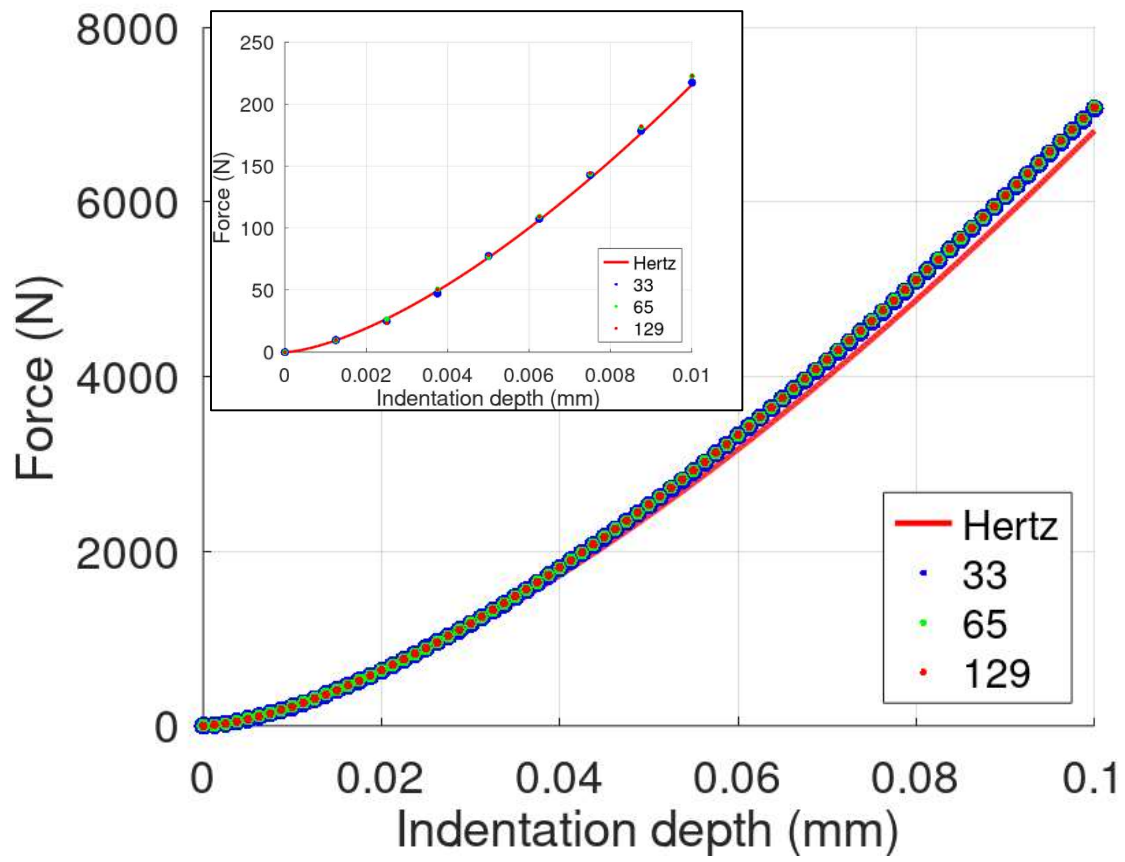


Figure 10 : Force-indentation depth curves from Small Strains simulations with 80 loading steps and a spatial resolution of 33^3 , 65^3 and 129^3 . The red continuous line represents the curve obtained with the Hertz theory.

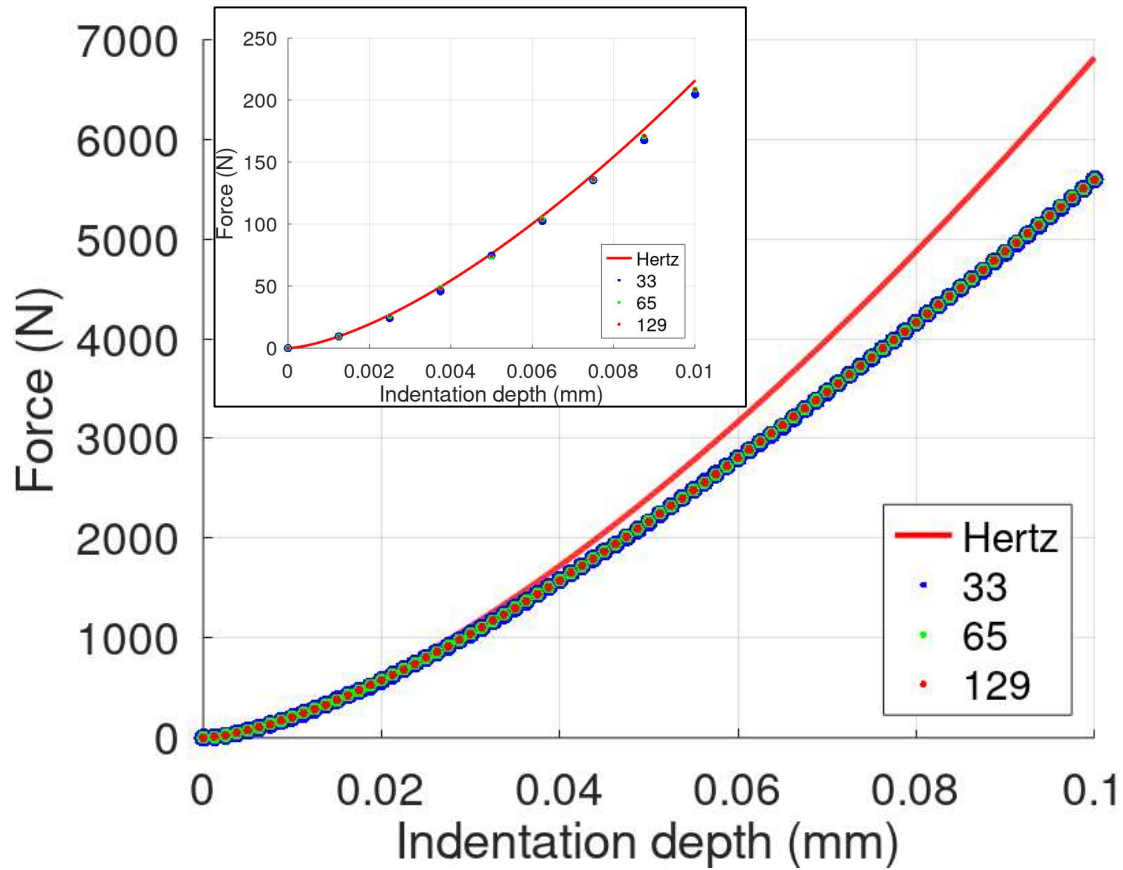


Figure 11 : Force-indentation depth curves from Finite Strains simulations with 80 loading steps and a spatial resolution of 33^3 , 65^3 and 129^3 . The red continuous line represents the curve obtained with the Hertz theory.

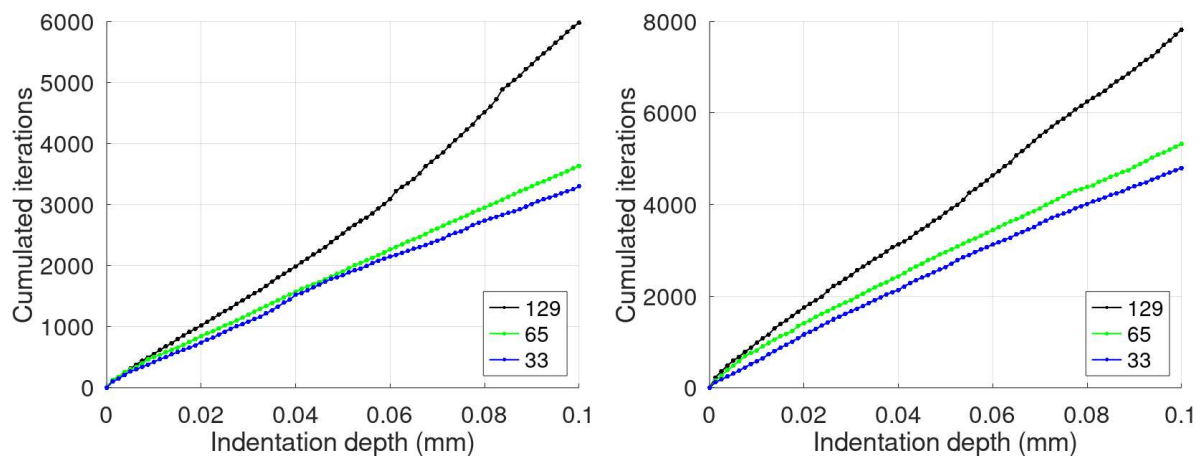


Figure 12 : Cumulated number of iterations for simulations with 80 loading steps and a spatial resolution of 33^3 , 65^3 and 129^3 , Small Strain case on the left side and Finite Strain case on the right side.

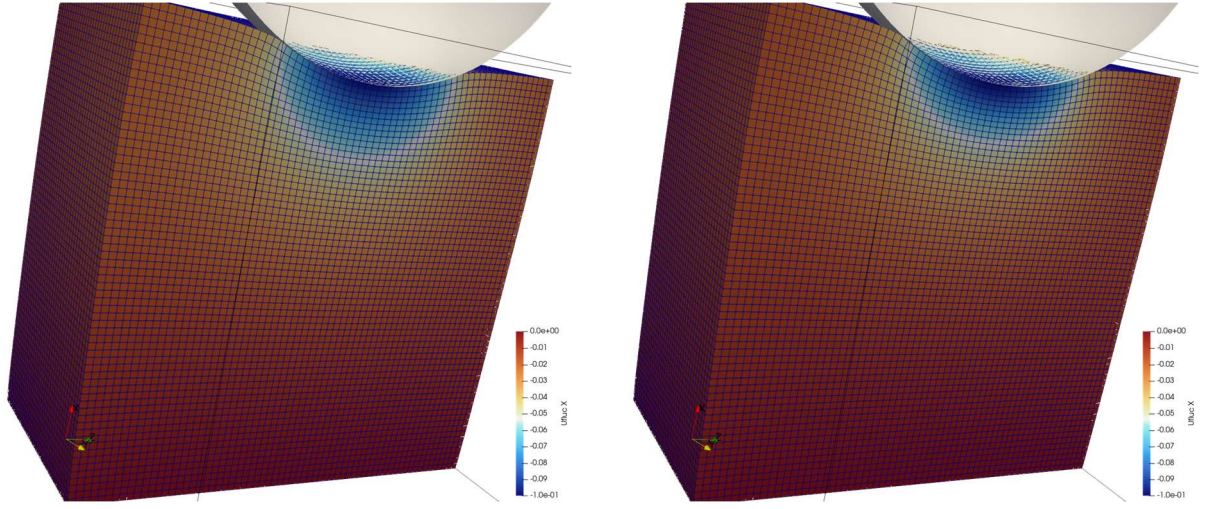


Figure 13 : Deformed configurations at the end of the loading for a resolution of 65^3 for Small Strain (left) and Finite Strains (right) simulations.

5.5: Discussion: minimization under inequality constraint

Following the discussion in section 4.3 looking at problems with local Dirichlet conditions as minimization problems subject to equality constraints, the present discussion considers a minimization problem with an inequality constraint given by the definition of the gap g (below $[g([\tilde{u}))]$ vanishes if $[\tilde{u}] = [0]$). For the SS case, the minimization problem (18) becomes:

$$\inf_{[\tilde{u}]} (J([\tilde{u}])) = \inf_{[\tilde{u}]} \left(\frac{1}{2} [\tilde{u}]^T \llbracket K \rrbracket [\tilde{u}] \right) \quad \text{with } [\tilde{u}] \text{ subject to } [g([\tilde{u}))] - [g_0] \geq 0 \quad (31)$$

As in section 4.3, the Lagrangian of this problem is considered leading to the definition of a saddle point.

$$\sup_{[f] \leq 0} \inf_{[\tilde{u}]} (J([\tilde{u}]) + [f]^T ([g([\tilde{u}))] - [g_0])) \quad (32)$$

Note that in that case, Lagrange multipliers are defined on the surface of potential contact S_1^1 and their admissible space is limited to negative values. The solution widely adopted by the contact mechanics community, is given by the Karush-Kuhn-Tucker conditions reported in a simplified way (i.e. assuming $g([\tilde{u}])$ linear).

$$\begin{cases} \begin{bmatrix} \llbracket K \rrbracket & \llbracket \partial_{\tilde{u}} g \rrbracket^T \\ \llbracket \partial_{\tilde{u}} g \rrbracket & \llbracket 0 \rrbracket \end{bmatrix} \begin{bmatrix} [\tilde{u}] \\ [f] \end{bmatrix} = \begin{bmatrix} [0] \\ [g_0] \end{bmatrix} \\ f_i \leq 0; \quad g_i - g_{0_i} \geq 0; \quad \text{and } f_i(g_i - g_{0_i}) = 0 \end{cases} \quad (33)$$

Index i runs over all the nodes (and components) of the potential contact surface S_1^1 . In practice, such problems can be solved using FE codes with an active set method: the first line is solved with Lagrange multipliers restricted to the point of a contact zone (active set), then the second line is used to detect where the constraints are violated and to update the contact zone (active set), and then return to the

first line to solve the linear problem with the updated contact zone (active set). The simulation of the spherical indentation reported above, demonstrates the ability of the proposed FFT-based solver to solve such minimization problems subject to inequality constraints. The methodology developed here for contact mechanics can be adapted to other physical equation subjected to inequality constraints.

6. Conclusion and future prospects

The starting point of the present work has been briefly described in section 3. The most important points are: the use of a displacement-based iterative algorithm, the efficient acceleration convergence technique used to accelerate the fixed-point algorithm, the use of DTTs to account for possibly non-periodic BCs per face and per component, and finally, the possibility to further explore the use of the TETRA2 finite difference scheme recently proposed by Finel [24] and its comparison with the HEX1 scheme.

Then, section 4 has proposed two simple modifications of the algorithm to account for local Dirichlet BCs (i.e. Dirichlet BCs that are not prescribed through DTTs on the faces of the unit-cell). The first one consists in a correction of the current unknown displacement field so that the local Dirichlet BCs are satisfied (i.e. just set the prescribed values in the current field). The second one consists in introducing reaction forces, at points where local Dirichlet are prescribed, to balance the stress divergence so that the equilibrium is systematically satisfied (i.e. just set null values in the current residual field $\mathbf{p}$). A non-trivial application is proposed through the loading of a half-CT(Compact Tension)-like specimen. The loading is applied on a single line of nodes inside the volume element, and a null displacement is applied on the ligament for the component 3. The rest of the surface is traction free (Neumann BC). While the HEX1 scheme (known for its possible instability associated to hourglass phenomenon) did not converge, results obtained with the TETRA2 scheme have been validated w.r.t. a FE simulation. To go beyond, the possibility to apply Dirichlet BCs to a single node has been explored, focusing on the TETRA2 scheme. It is emphasized, and explained from Finel description [24], that it is impossible to apply the displacement to a single node. Hence, the first alternative approach applies the Dirichlet BCs to the center of a voxel, so that a linear relationship is imposed between the 8 nodes of the voxel. The second approach prescribes the displacement of a single node but redistribute the reaction force on neighboring nodes. As reaction forces and Lagrange multipliers are closely related, this last approach could be referred to as “diffuse” Lagrange multipliers. The two methods have been tested and compared successfully. At the end of section 4, the local equations used to introduce the algorithm are discussed with the viewpoint of minimization with equality constraints and the introduction of Lagrange multipliers. The conclusion of this section is that the proposed FFT-based solver has demonstrated its ability to solve minimization with equality constraints, including relations between displacements of different nodes. To the knowledge of the author, the concept of “diffuse” Lagrange multipliers is also proposed originally.

Finally, the question of minimization problems with inequality constraints is investigated with a focus on the simulation of contact mechanics through a simple application (a rigid spherical indenter on a cube volume element assuming frictionless contact). The modification of the previous algorithm proposed to apply local Dirichlet BCs is modified to incorporate a so-called active set method to deal with the evolution of the contact zone. The active set method consists simulating the problem with Dirichlet BCs for a given contact zone, then verify where the contact conditions are violated, then modify the contact zone (i.e. the active set) and re-run the simulation with local Dirichlet BCs but with the new contact zone. This procedure is run iteratively until stability of the contact zone. This active set method is closely introduced within the accelerated fixed-point algorithm. The algorithm is then

proposed in the context of small strain assumption but also in the context of finite strain. The robustness of the method has been established through different sensitivity analysis w.r.t. spatial resolution and loading discretization. For small (indentation depth / sphere radius) ratio corresponding to the validity domain of the Hertz theory, the SS and FS implementations are very close to the results given by the Hertz theory, validating at least partially the two implementations. When increasing the ratio, the curves obtained with SS and FS depart from each other, demonstrating the importance of taking into account the FS framework instead of the SS assumption.

As a future prospect, the present work widely opens the door of structural analysis to FFT-based solvers. In addition, if two different finite difference schemes (HEX1 and TETRA2) are used, it must not hide the ability of the method to account for various types of finite element discretization (see for instance Schneider [22] or Ladecký [45]). Similarly, if the method is proposed with a regular grid discretization, it must be emphasized that a grid adaptation can also be taken into account (see the works of Zecevic [46], Bellis [47] or Bignonnet [48]). Note that composite voxels [1] could also be thought to apply BCs in the case of immersed boundaries. At the end, gathering all these advances in a single parallel implementation, for example the AMITEX* code, a partial re-writing of the AMITEX code [14] developed by the author, could be a very nice project.

In term of distributed memory parallel implementation, it must be emphasized that for “strongly applied” Dirichlet BCs (see section 4.1) the parallel implementation in a 2D domain decomposition (pencil decomposition), as done in AMITEX/AMITEX* (see Amouzou-Adoun et al. [1]) using the library 2decomp&fft [43], is quite straightforward. The remark is the same for the algorithm proposed for indentation and the code used in the present paper is already parallel. On the other hand, for “weakly” or “smoothly” applied BCs (see section 4.2), as the conditions are distributed over several nodes that can be located on different domains, the implementation is a bit more complex. As a proof of concept, the implementation of these non-local BCs is still limited to single processor simulations, the parallel extension being a short-term project.

Finally, if the methodology proposed to solve minimization problems with equality or inequality constraints is introduced here in the framework of local continuum mechanics, the method is completely general and can be applied to various set of equations related to different physics, or non-local equations in mechanics.

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- [1] Yaovi Armand Amouzou-Adoun, Cédric Flageul, Yushan Wang, and Lionel Gelebart. A robust and versatile parallel fft-based mechanical solver for general non-periodic and periodic boundary conditions. *submitted to CMAME, available at SSRN: <https://ssrn.com/abstract=7075197> or <http://dx.doi.org/10.2139/ssrn.7075197>*, 2026.
- [2] H. Moulinec and P. Suquet. A numerical method for computing the overall response of nonlinear composites with complex microstructure. *Computer Methods In Applied Mechanics and Engineering*, 157(1-2):69–94, April 1998.
- [3] Matti Schneider. A review of nonlinear fft-based computational homogenization methods. *Acta Mechanica*, 232(6):2051–2100, 2021.
- [4] Sergio Lucarini, Manas Vijay Upadhyay, and Javier Segurado. Fft based approaches in micromechanics: fundamentals, methods and applications. *Modelling and Simulation in Materials Science and Engineering*, 2021.
- [5] Christian Gierden, Julian Kochmann, Johanna Waimann, Bob Svendsen, and Stefanie Reese. A review of fe-fft-based two-scale methods for computational modeling of microstructure evolution and macroscopic material behavior. *Archives of Computational Methods in Engineering*, 29(6):4115–4135, 2022.
- [6] D. J. Eyre and G. W. Milton. A fast numerical scheme for computing the response of composites using grid refinement. *European Physical Journal-applied Physics*, 6(1):41–47, April 1999.
- [7] J. C. Michel, H. Moulinec, and P. Suquet. A computational scheme for linear and non-linear composites with arbitrary phase contrast. *International Journal For Numerical Methods In Engineering*, 52(1-2):139–158, September 2001.
- [8] V. Monchiet and G. Bonnet. A polarization-based fft iterative scheme for computing the effective properties of elastic composites with arbitrary contrast. *International Journal For Numerical Methods In Engineering*, 89(11):1419–1436, March 2012.
- [9] H. Moulinec and F. Silva. Comparison of three accelerated fft-based schemes for computing the mechanical response of composite materials. *International Journal for Numerical Methods in Engineering*, 97(13):960–985, 2014.
- [10] J. Zeman, J. Vondrejč, J. Novak, and I. Marek. Accelerating a fft-based solver for numerical homogenization of periodic media by conjugate gradients. *Journal of Computational Physics*, 229(21):8065–8071, October 2010.
- [11] S. Brisard and L. Dormieux. Fft-based methods for the mechanics of composites: A general variational framework. *Computational Materials Science*, 49(3):663–671, September 2010.
- [12] L. Gélébart and R. Mondon-Cancel. Non-linear extension of fft-based methods accelerated by conjugate gradients to evaluate the mechanical behavior of composite materials. *Computational Materials Science*, 77(0):430–439, September 2013.
- [13] M. Kabel, T. Böhlke, and M. Schneider. Efficient fixed point and newton-krylov solvers for fft-based homogenization of elasticity at large deformations. *Computational Mechanics*, 54(6):1497–1514, 2014.
- [14] Lionel Gélébart. <https://amitexfftp.github.io/amitex/index.html>. 2022.

- [15] Y. Chen, L. Gélébart, C. Chateau, M. Bornert, C. Sauder, and A. King. Analysis of the damage initiation in a sic/sic composite tube from a direct comparison between large-scale numerical simulation and synchrotron x-ray micro-computed tomography. *Int. J. Solids Struct.*, 161:111 – 126, 2019.
- [16] Cast3m, ww-cast3m.cea.fr.
- [17] D.G. Anderson. Iterative procedures for nonlinear integral equations. *Journal of the ACM (JACM)*, 12(4):547–560, 1965.
- [18] S. Brisard and L. Dormieux. Combining galerkin approximation techniques with the principle of hashin and shtrikman to derive a new fft-based numerical method for the homogenization of composites. *Computer Methods In Applied Mechanics and Engineering*, 217:197–212, 2012.
- [19] Jaroslav Vondrej, Jan Zeman, and Ivo Marek. An fft-based galerkin method for homogenization of periodic media. *Computers & Mathematics with Applications*, 68(3):156 – 173, 2014.
- [20] Wiegmann A. Fast poisson, fast helmholtz and fast linear elastostatic solvers on rectangular parallelepipeds. Technical report, Lawrence Berkeley National Lab. (LBNL), Berkeley, CA (United States), 1999.
- [21] F. Willot. Fourier-based schemes for computing the mechanical response of composites with accurate local fields. *Comptes Rendus Mécanique*, 343(3):232 – 245, 2015.
- [22] M. Schneider, D. Merkert, and M. Kabel. Fft-based homogenization for microstructures discretized by linear hexahedral elements. *International Journal for Numerical Methods in Engineering*, 109(10):1461–1489, 2017.
- [23] Lionel Gélébart. Fft-based simulations of heterogeneous conducting materials with combined non-uniform neumann, periodic and dirichlet boundary conditions. *European Journal of Mechanics - A/Solids*, 105:105248, 2024.
- [24] A. Finel. A tetrahedron-based discretization for fft-based computational homogenization with smooth solution fields. *Computer Methods in Applied Mechanics and Engineering*, 436:117703, 2025.
- [25] Lionel Gélébart. A modified fft-based solver for the mechanical simulation of heterogeneous materials with dirichlet boundary conditions. *Comptes Rendus. Mécanique*, 348(8-9):693–704, 2020.
- [26] Noé Brice Nkoumbou Kaptchouang and Lionel Gélébart. Multiscale coupling of fft-based simulations with the ldc approach. *Computer Methods in Applied Mechanics and Engineering*, 394:114921, 2022.
- [27] Miroslav Zecevic and Ricardo A. Lebensohn. Extended fft-based micromechanical formulation to consider general non-periodic boundary conditions. *International Journal of Solids and Structures*, page 113225, 2025.
- [28] V. Monchiet and G. Bonnet. Fft based iterative schemes for composite conductors with uniform boundary conditions. *European Journal of Mechanics - A/Solids*, 103:105146, 2024.
- [29] Hannes Grimm-Strele and Matthias Kabel. Fft-based homogenization with mixed uniform boundary conditions. *Int J Numer Methods Eng*, 122(23):7241–7265, December 2021.

- [30] Léo Morin and Joseph Paux. A fast numerical method for the conductivity of heterogeneous media with dirichlet boundary conditions based on discrete sine-cosine transforms. *Computer Methods in Applied Mechanics and Engineering*, 421:116772, 2024.
- [31] Lennart Risthaus and Matti Schneider. Imposing different boundary conditions for thermal computational homogenization problems with fft- and tensor-train-based green's operator methods. *Int J Numer Methods Eng*, n/a(n/a):e7423, January 2024.
- [32] Joseph Paux, Léo Morin, and Lionel Gélébart. A discrete sine-cosine transforms galerkin method for the conductivity of heterogeneous materials with mixed dirichlet/neumann boundary conditions. *Int J Numer Methods Eng*, n/a(n/a):e7615, November 2024.
- [33] Lennart Risthaus and Matti Schneider. Fft-based computational micromechanics with dirichlet boundary conditions on the rotated staggered grid. *Int J Numer Methods Eng*, n/a(n/a):e7569, July 2024.
- [34] Joseph Paux, Léo Morin, Lionel Gélébart, and Abdoul Magid Amadou Sanoko. A discrete sine-cosine based method for the elasticity of heterogeneous materials with arbitrary boundary conditions. *Computer Methods in Applied Mechanics and Engineering*, 433:117488, 2025.
- [35] X. Kleber P. Sainsot F. Ville L. Fourel, J.-P. Noyel. Green-fft model for 3d contacts considering microstructure and defects. *Mechanics & Industry*, 26(10), 2025.
- [36] Lucas Frérot, Marc Bonnet, Jean-François Molinari, and Guillaume Anciaux. A fourier-accelerated volume integral method for elastoplastic contact. *Computer Methods in Applied Mechanics and Engineering*, 351:951–976, 2019.
- [37] Q. Jane Wang, Linlin Sun, Xin Zhang, Shuangbiao Liu, and Dong Zhu. Fft-based methods for computational contact mechanics. *Frontiers in Mechanical Engineering*, Volume 6 - 2020, 2020.
- [38] Lionel Gélébart. A simple extension of FFT-based methods to strain gradient loadings - Application to the homogenization of beams and plates with linear and non-linear behaviors. *Journal of Theoretical, Computational and Applied Mechanics*, June 2022.
- [39] Lionel Gélébart. An accurate and robust fft-based solver for transient diffusion in heterogeneous materials. *Comptes Rendus. Mécanique*, 353:113–125, 2025.
- [40] Isabelle Ramière and Thomas Helfer. Iterative residual-based vector methods to accelerate fixed point iterations. *Computers & Mathematics with Applications*, 70(9):2210–2226, 2015.
- [41] Lennart Risthaus and Matti Schneider. Imposing dirichlet boundary conditions directly for fft-based computational micromechanics. *Computational Mechanics*, 2024.
- [42] M. Frigo and S. G. Johnson. The design and implementation of fftw3. *Proceedings of the IEEE*, 93(2):216–231, 2005.
- [43] Stefano Rolfo, Cédric Flageul, Paul Bartholomew, Filippo Spiga, and Sylvain Laizet. The 2decomp&fft library: an update with new cpu/gpu capabilities. *Journal of Open Source Software*, 8(91):5813, 2023.
- [44] Vladislav Yastrebov. Numerical methods in contact mechanics. Wiley, February 2013.
- [45] Martin Ladecký, Richard J. Leute, Ali Falsafi, Ivana Pultarová, Lars Pastewka, Till Junge, and Jan Zeman. An optimal preconditioned fft-accelerated finite element solver for homogenization. *Applied Mathematics and Computation*, 446:127835, 2023.

- [46] Miroslav Zecevic, Ricardo A. Lebensohn, and Laurent Capolungo. Achieving geometric accuracy in fft-based micromechanical models using conformal grid. *Mechanics of Materials*, page 105512, 2025.
- [47] Cédric Bellis and Renaud Ferrier. Numerical homogenization by an adaptive fourier spectral method on non-uniform grids using optimal transport. *Computer Methods in Applied Mechanics and Engineering*, 419:116658, 2024.
- [48] François Bignonnet, Martin Ladecký, Ivana Pultarová, and Jan Zeman. Fourier-based computational micromechanics on boundary-conforming transformed grids. *Comptes Rendus. Mécanique*, 354:227–256, 2026.